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                 REGISTRY
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NEWS 11 MAY 11 STN on the Web enhanced
NEWS 12 MAY 11
                 BEILSTEIN substance information now available on
                 STN Easy
                 DGENE, PCTGEN and USGENE enhanced with increased
NEWS 13
         MAY 14
                 limits for exact sequence match searches and
                 introduction of free HIT display format
NEWS 14
         MAY 15
                 INPADOCDB and INPAFAMDB enhanced with Chinese legal
                 status data
NEWS 15
         MAY 28 CAS databases on STN enhanced with NANO super role in
                 records back to 1992
NEWS 16
         JUN 01 CAS REGISTRY Source of Registration (SR) searching
                 enhanced on STN
NEWS 17
         JUN 26 NUTRACEUT and PHARMAML no longer updated
NEWS 18
                 IMSCOPROFILE now reloaded monthly
         JUN 29
         JUN 29 EPFULL adds Simultaneous Left and Right Truncation
NEWS 19
                 (SLART) to AB, MCLM, and TI fields
NEWS 20
         JUL 09 PATDPAFULL adds Simultaneous Left and Right
                 Truncation (SLART) to AB, CLM, MCLM, and TI fields
NEWS 21
         JUL 14 USGENE enhances coverage of patent sequence location
                 (PSL) data
NEWS 22
         JUL 27
                 CA/CAplus enhanced with new citing references
NEWS 23
         JUL 16
                 GBFULL adds patent backfile data to 1855
NEWS 24
         JUL 21
                 USGENE adds bibliographic and sequence information
                 EPFULL adds first-page images and applicant-cited
NEWS 25
         JUL 28
                 references
NEWS 26 JUL 28
                 INPADOCDB and INPAFAMDB add Russian legal status data
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=> fil reg
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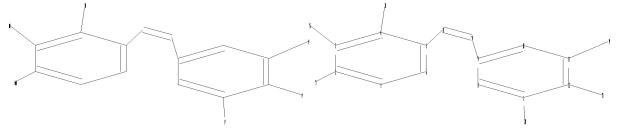
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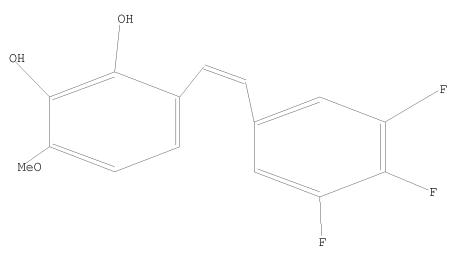
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chain nodes :
13  14  15  16  17  18  19  20
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12
chain bonds :
2-17  3-16  4-15  5-13  7-20  9-14  11-19  12-18  13-14
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  8-9  9-10  10-11  11-12
exact/norm bonds :
3-16  4-15
exact bonds :
2-17  5-13  7-20  9-14  11-19  12-18  13-14
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  8-9  9-10  10-11  11-12
```

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS

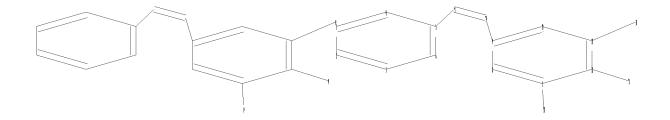
L1 STRUCTURE UPLOADED

=> d L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> Uploading C:\Program Files\Stnexp\Queries\10-790662 a.str



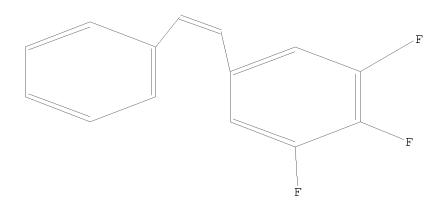
chain nodes :
13 14 15 16 17
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
5-13 7-17 9-14 11-16 12-15 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact bonds :
5-13 7-17 9-14 11-16 12-15 13-14
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS

L2 STRUCTURE UPLOADED

=> d L2 HAS NO ANSWERS L2 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 12
SAMPLE SEARCH INITIATED 09:43:25 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 62 TO ITERATE

100.0% PROCESSED 62 ITERATIONS 8 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

PROJECTED ITERATIONS: 768 TO 1712

PROJECTED ANSWERS: 8 TO 329

L3 8 SEA SSS SAM L2

=> d scan

L3 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, [(1E)-2-(2-chlorophenyl)ethenyl]pentafluoro- (9CI)

MF C14 H6 Cl F5

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):7

L3 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Acetamide, N-[(2S,11aS)-2,3,5,10,11,11a-hexahydro-5,11-dioxo-7-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-lH-pyrrolo[2,1-c][1,4]benzodiazepin-2-yl]-2-methoxy-

MF C23 H18 F5 N3 O4

Absolute stereochemistry.

Double bond geometry unknown.

L3 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

Benzene, 1,1'-[1-[(4-methylphenyl)sulfonyl]-1,2-ethenediyl]bis[2,3,4,5,6-pentafluoro-(9CI)ΙN

C21 H8 F10 O2 S MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 REGISTRY COPYRIGHT 2009 ACS on STN

Benzene, 1-ethyl-3, 4, 5-trifluoro-2-[(1E)-2-(3,4,5-trifluorophenyl)ethenyl]-IN

MF C16 H10 F6

8 ANSWERS L3 REGISTRY COPYRIGHT 2009 ACS on STN

Benzamide, 4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-N-[3-ΙN (phosphonooxy)propyl]-

C18 H15 F5 N O5 P MF

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- REGISTRY COPYRIGHT 2009 ACS on STN L3 8 ANSWERS
- 2-Butenedinitrile, 2,3-bis(pentafluorophenyl)-, radical ion(1-), IN vanadium(2+), (2E)- (9CI) C16 F10 N2 . 1/2 V
- MF
- COM, RIS CI

●1/2 V(II) 2+

L3 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 5-[(12)-1-(chloromethyl)-2-(4-fluorophenyl)ethenyl]-1,2,3-trifluoro-

MF C15 H9 Cl F4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1-[(1E)-2-(2,4-dimethoxyphenyl)ethenyl]-2,3,4,5,6-pentafluoro-MF C16 H11 F5 O2

ALL ANSWERS HAVE BEEN SCANNED

=> s 12 full

FULL SEARCH INITIATED 09:48:03 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1496 TO ITERATE

100.0% PROCESSED 1496 ITERATIONS

201 ANSWERS

SEARCH TIME: 00.00.01

L4 201 SEA SSS FUL L2

=> d scan

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

MF C16 F10 N2

CI COM, RIS

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):200 $\verb|'200|'$ IS NOT VALID HERE

To display more answers, enter the number of answers you would like to see. To end the display, enter "NONE", "N", "0", or "END". HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):200

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-

MF C22 H8 F10

201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN L4

ΙN Benzeneacetonitrile, α -[[4-(cyanomethy1)-2,3,5,6tetrafluorophenyl](2,3,4,5,6-pentafluorophenyl)methylene]-2,3,4,5,6pentafluoro-, compd. with cyclohexanamine (1:1) C23 H2 F14 N2 . C6 H13 N

MF

CM1

CM2

IN Benzene-1,3-d2, 2-[(1E)-2-[2-(ethyl-2-d)-4,5,6-trifluorophenyl-3-d]ethenyl]-4,5,6-trifluoroMF C16 H6 D4 F6

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzene, 1,2,3-trifluoro-5-[(1E)-2-(3-fluoro-4-methoxyphenyl)ethenyl]MF C15 H10 F4 O

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzene, 1,2-dimethyl-, compd. with
(E,E)-1,4-bis[2-(pentafluorophenyl)ethenyl]benzene (1:1) (9CI)
MF C22 H8 F10 . C8 H10

CM 1

CM 2

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzoic acid, pentafluoro-, 1,2-bis(pentafluorophenyl)-1,2-ethenediyl ester, (Z)- (9CI)

MF C28 F20 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

IN Benzene, 1,2,3-trifluoro-5-[(1Z)-2-(4-methoxy-3-nitrophenyl)ethenyl]-MF C15 H10 F3 N O3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-, (4S,4aS,5aR,12aS)-

MF C29 H23 F5 N2 O7

Absolute stereochemistry.

Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Indene-1,3(2H)-dione, 2-[[4-[2-(2,3,4,5,6-pentafluorophenyl)-2-phenylethenyl]phenyl]methylene]-

MF C30 H15 F5 O2

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzene, pentafluoro[(1E)-2-(4-methylphenyl)ethenyl]- (9CI)
MF C15 H9 F5

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Bicyclo[2.2.2]octane, 1-bromo-4-[(1E)-2-[4-[(1E)-2-(3,4,5-trifluorophenyl)ethenyl]phenyl]ethenyl]MF C24 H22 Br F3

PAGE 2-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzene, 1,1'-[(1Z,2Z)-1,2-bis(phenylmethylene)-1,2-

ethanediyl]bis[2,3,4,5,6-pentafluoro- (9CI)

MF C28 H12 F10

L4

201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN Benzoic acid, 3,3'-[(pentafluorophenyl)ethenylidene]bis[5-chloro-6-methoxy-ΙN (9CI)

MF C24 H13 C12 F5 O6

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN L4

Benzenemethanol, 2,3,4,5,6-pentafluoro- α -[(2,3,4,5,6-ΙN pentafluorophenyl)methylene]-, sodium salt (1:1)

C14 H2 F10 O . Na MF

Na

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4

201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN 2-Thiophenecarboxamide, N-[(2S,11aS)-2,3,5,10,11,11a-hexahydro-5,11-dioxo-ΙN 7-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-1H-pyrrolo[2,1c][1,4]benzodiazepin-2-y1]-

C25 H16 F5 N3 O3 S MF

Absolute stereochemistry. Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-(3-nitrophenyl)]-ΙN

C14 H6 F5 N O2 MF

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3,4-tetrafluoro-5-[2-(4-methoxyphenyl)ethenyl]-

MF C15 H10 F4 O

$$\begin{array}{c|c} F & CH & CH \\ \hline F & F & OMe \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,1'-(1,2-dibromo-1,2-ethenediyl)bis[2,3,4,5,6-pentafluoro-

MF C14 Br2 F10

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenemethanol, α -[(2,3,4,5,6-pentafluorophenyl)methylene]-

MF C14 H7 F5 O

CI COM

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetaldehyde, $\alpha-[(1,3-\text{dihydro}-5-\text{methoxy}-1,3,3-\text{trimethylspiro}[2H-\text{indole}-2,3'-[3H]naphth[2,1-b][1,4]oxazin]-5'-yl)methylene]-2,3,4,5,6-pentafluoro-$

MF C32 H23 F5 N2 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetonitrile, α -[[4-(cyanomethyl)-2,3,5,6-tetrafluorophenyl](2,3,4,5,6-pentafluorophenyl)methylene]-2,3,4,5,6-pentafluoro-, compd. with 1-propanamine (1:1)

MF C23 H2 F14 N2 . C3 H9 N

CM 1

CM 2

 $_{\mathrm{H_3C-CH_2-CH_2-NH_2}}$

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

Double bond geometry as shown.

PAGE 1-A

201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN L4

Benzene, 5-[(1Z)-2-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-ΙN methoxyphenyl]ethenyl]-1,2,3-trifluoro-

C21 H25 F3 O2 Si MF

Double bond geometry as shown.

MeO
$$\frac{\overline{Z}}{\overline{Bu-t}}$$
 F F $\overline{Bu-t}$ F

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

Benzene, 1,1'-(1,2-ethenediyl) bis [2,3,4,5,6-pentafluoro-, (E)-, compd.]ΙN with (E)-1,1'-(1,2-ethenediy1)bis[benzene] (1:1) (9CI) C14 H12 . C14 H2 F10

MF

CM 1

$$\begin{matrix} F & & F \\ F & & F \\ F & & F \end{matrix}$$

CM2

Double bond geometry as shown.

$$\Pr_{\mathsf{Ph}} \overset{\mathsf{E}}{\longrightarrow} \mathsf{Ph}$$

REGISTRY COPYRIGHT 2009 ACS on STN L4201 ANSWERS

ΙN Benzene, pentafluoro[2-[2,3,4,5-tetrafluoro-6-

[(methylthio)methyl]phenyl]ethenyl]-, (E)- (9CI) C16 H7 F9 S

MF

Double bond geometry as shown.

$$\begin{matrix} F & & F \\ F & & & F \\ \hline F & & & SMe & F \\ \end{matrix}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2009 ACS on STN 201 ANSWERS L4

Benzene, 1,2,3-trifluoro-5-[(1Z)-2-(4-methoxy-2-nitrophenyl)ethenyl]-ΙN

C15 H10 F3 N O3 MF

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3,4,5-pentafluoro-6-[2-[(4-methylphenyl)sulfonyl]-2phenylethenyl]-

MF C21 H13 F5 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanol, 2-[methyl[4-[2-(2,3,4,5-tetrafluoro-6-

nitrophenyl)ethenyl]phenyl]amino]-

MF C17 H14 F4 N2 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, pentafluoro(3,3,3-trifluoro-2-phenyl-1-propenyl)-, (E)- (9CI)

MF C15 H6 F8

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Bicyclo[2.2.2]octane, 1-methoxy-4-[(1E)-2-[4-[(1E)-2-(3,4,5-

trifluorophenyl)ethenyl]phenyl]ethenyl]-

MF C25 H25 F3 O

Double bond geometry as shown.

PAGE 1-A



L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, 2,3,4,5,6-pentafluoro- α -(phenylmethylene)-

MF C15 H7 F5 O2

$$\begin{array}{c|c} F & CO_2H \\ \hline C & CH-Ph \\ \hline F & F \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3-trifluoro-5-[(1E)-2-(4-methoxyphenyl)ethenyl]-

MF C15 H11 F3 O

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, 2,3,4,5,6-pentafluoro- α -[(2,3,4,5,6-pentafluorophenyl)methylene]-, compd. with phenylmethyl carbamimidothioate (1:1)

MF C15 H2 F10 O2 . C8 H10 N2 S

CM 1

СМ 2

$$\begin{array}{c} \text{NH} \\ || \\ \text{H}_2 \text{N-C-S-CH}_2 \text{-Ph} \end{array}$$

REGISTRY COPYRIGHT 2009 ACS on STN 201 ANSWERS L4

Benzene, 1-[2-(3,5-dimethoxy-4-propylphenyl)ethenyl]-2,3,4,5,6-pentafluoro-ΙN MF C19 H17 F5 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

2-Butenedinitrile, 2,3-bis(pentafluorophenyl)-, radical ion(1-), ΙN vanadium(2+), (2E)-, compd. with tetrahydrofuran (9CI) C16 F10 N2 . \times C4 H8 O . 1/2 V

MF

CM 1

ullet1/2 V(II)²⁺

CM 2



L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenamine, N-[4-(2,2-diphenylethenyl)phenyl]-4-ethyl-3-methyl-N-[4-[2-(2,3,4,5,6-pentafluorophenyl)-2-phenylethenyl]phenyl]-

MF C49 H36 F5 N

$$\begin{array}{c|c} & & & \\ F & & \\ F & & \\ \hline F & & \\ \hline F & & \\ \hline CH & CPh_2 & \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,1'-(12)-1,2-ethenediylbis[2,3,4,5,6-pentafluoro-(9CI)

MF C14 H2 F10

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1-[2-[3,5-dimethoxy-4-(1-methylethyl)phenyl]ethenyl]-2,3,4,5,6-pentafluoro-

MF C19 H17 F5 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3-trifluoro-5-[(1E)-2-[4-(trans-4propylcyclohexyl)phenyl]ethenyl]-

MF C23 H25 F3

Relative stereochemistry. Double bond geometry as shown.

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

MF C18 H6 F10 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenemethanamine, 2,3,4,5,6-pentafluoro- α -[nitro(2,3,4,5,6-pentafluorophenyl)methylene]-

MF C14 H2 F10 N2 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzaldehyde, 4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-

MF C15 H7 F5 O

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Naphthalene, 2-[(1E)-2-(3,4,5-trifluorophenyl)ethenyl]-MF C18 H11 F3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 1,3-Benzodioxole, 5-[2-(pentafluorophenyl)ethenyl]-, (E)- (9CI) MF C15 H7 F5 O2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, 3,4,5-trifluoro- α -[(4-methoxyphenyl)methylene]-, (α E)-

MF C16 H11 F3 O3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1-[2-(2,6-dichlorophenyl)-1-[(4-methylphenyl)sulfonyl]ethenyl]-2,3,4,5,6-pentafluoro-

MF C21 H11 C12 F5 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, pentafluoro[2-(2,3,5,6-tetrafluoro-4-nitrophenyl)ethenyl]- (9CI)

MF C14 H2 F9 N O2

$$CH$$
 CH
 CH
 F
 F
 F
 F

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, [(1Z)-(1,2-diphenylethenyl)]pentafluoro- (9CI)

MF C20 H11 F5

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetonitrile, $\alpha-[[4-[3,5-bis(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methylene]-3,4,5-trifluoro-$

MF C20 H8 F9 N3

$$F_3$$
C CH CH CH F F

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,1'-(1E)-1,2-ethenediylbis[3,4,5-trifluoro-(9CI)

MF C14 H6 F6

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1-[2-(4-methoxyphenyl)ethenyl]-4-[2-(pentafluorophenyl)ethenyl]-, (E,E)- (9CI)

MF C23 H15 F5 O

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Acrylonitrile, 2,3-bis(pentafluorophenyl)-, (E)- (8CI)

MF C15 H F10 N

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,2-Benzenediol, 3-methoxy-6-[(1Z)-2-(3,4,5-trifluorophenyl)]ethenyl]-

MF C15 H11 F3 O3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Butenedinitrile, 2,3-bis(pentafluorophenyl)-, (2E)- (9CI)

MF C16 F10 N2

L4201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

Benzeneacetonitrile, $\alpha-[[4-(cyanomethy1)-2,3,5,6-$ ΙN tetrafluorophenyl](2,3,4,5,6-pentafluorophenyl)methylene]-2,3,4,5,6pentafluoro-, compd. with N,N-diethylethanamine (1:1) C23 H2 F14 N2 . C6 H15 N

MF

CM

СМ 2

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ΙN INDEX NAME NOT YET ASSIGNED

MF (C20 H18 O3 . C14 H7 F5 . C12 F10)x

CI PMS

> CM1

CM 2

CM 3

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenamine, N,N-dimethyl-4-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-

MF C16 H12 F5 N

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Diazene, 1-[2-[(1Z)-1,2-bis(2,3,4,5,6-pentafluorophenyl)ethenyl]-3,5-dichlorophenyl]-2-phenyl-, (1E)-MF C26 H8 Cl2 F10 N2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzenamine, 2-methoxy-5-[(1E)-2-(3,4,5-trifluorophenyl)ethenyl]MF C15 H12 F3 N O

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1-[(1E)-2-(2,4-dimethoxyphenyl)ethenyl]-2,3,4,5,6-pentafluoro-

MF C16 H11 F5 O2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Indene-1,3(2H)-dione, 2-[2,3-dihydro-3-oxo-2-[[4-[2-(2,3,4,5,6-pentafluorophenyl)-2-phenylethenyl]phenyl]methylene]-1H-inden-1-ylidene]-

MF C39 H19 F5 O3

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, [2-(4-bromophenyl)ethenyl]pentafluoro-, (2)- (9CI)

MF C14 H6 Br F5

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Adenosine, 5'-0-[hydroxy[3-[[4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl])ethenyl]benzoyl]amino]propoxy]phosphinyl]thymidylyl- $(3'\rightarrow5')-2'$ -deoxyguanylyl- $(3'\rightarrow5')-2'$ -deoxygutidylyl- $(3'\rightarrow5')-2'$ -deoxyguanylyl- $(3'\rightarrow5')-2'$ -deoxycytidylyl-

 $(3'\rightarrow5')-2'-\text{deoxy}-$ MF C76 H87 F5 N24 O38 P6

Absolute stereochemistry.

PAGE 2-B

___NH2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 2-Butenedinitrile, 2,3-bis(pentafluorophenyl)-, radical ion(1-), vanadium(2+), (2E)-, compd. with acetonitrile (9CI) C16 F10 N2 . \times C2 H3 N . 1/2 V

MF

СМ 1

●1/2 V(II) 2+

СМ

 $H3C-C \equiv N$

L4201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzenamine, N,N-dimethyl-4-[2-(2,3,4,5-tetrafluoro-6-nitrophenyl)ethenyl]-MF C16 H12 F4 N2 O2

$$\begin{array}{c|c} F \\ \hline F \\ \hline NO_2 \\ \hline \end{array} \quad \begin{array}{c} NMe_2 \\ \hline \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-(4-methoxyphenyl)ethenyl]MF C15 H9 F5 O

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Urea, N-[(2S,11aS)-2,3,5,10,11,11a-hexahydro-5,11-dioxo-7-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-1H-pyrrolo[2,1-c][1,4]benzodiazepin-2-yl]-N'-(3-methoxyphenyl)-

MF C28 H21 F5 N4 O4

Absolute stereochemistry.

Double bond geometry unknown.

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3-trifluoro-5-[(1E)-2-(3,4,5-trimethylphenyl)ethenyl]-

MF C17 H15 F3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, pentafluoro[3,3,3-trifluoro-2-phenyl-1-(trifluoromethyl)-1 propenyl]-, (Z)- (9CI)

MF C16 H5 F11

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzene, 1,1'-(1,2-ethenediyl)bis[2,3,4,5-tetrafluoro-, (E)- (9CI)
MF C14 H4 F8

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzenemethanol, 2,3,4,5,6-pentafluoro- α -[(2,3,4,5,6-

pentafluorophenyl)methylene]-

MF C14 H2 F10 O

CI COM

- 201 ANSWERS L4REGISTRY COPYRIGHT 2009 ACS on STN
- Poly[[1,1'-biphenyl]-4,4'-diyl[(1Z)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(pentafluorophenyl)-1,2-bis(peΙN ethenediyl]] (9CI)
- MF(C26 H8 F10)n
- PMS CI

PAGE 1-A

$$\begin{bmatrix} F & F & C & R \\ F & F & C & R \end{bmatrix}$$

PAGE 2-A

- 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN L4
- Benzeneacetonitrile, $\alpha-[[4-(cyanomethy1)-2,3,5,6-$ ΙN tetrafluorophenyl](2,3,4,5,6-pentafluorophenyl)methylene]-2,3,4,5,6-pentafluoro-, compd. with N-(1-methylethyl)-2-propanamine (1:1) C23 H2 F14 N2 . C6 H15 N
- MF

СМ 1

CM 2

i-Pr-NH-Pr-i

L4

201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN Phosphine, 1,1'-[1,4-phenylenebis[(1E,3E)-3-(2,3,4,5,6-pentafluorophenyl)-4-phenyl-1,3-butadiene-4,1-diyl]]bis[1,1-diphenyl-ΙN

MF C62 H38 F10 P2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4REGISTRY COPYRIGHT 2009 ACS on STN 201 ANSWERS

Benzene, 1,2,3-trifluoro-5-[(1Z)-2-(4-methoxyphenyl)ethenyl]-ΙN

MF C15 H11 F3 O

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Cinnoline, 8-[1,2-bis(2,3,4,5,6-pentafluorophenyl)ethenyl]-6-chloro-2-(4-chlorophenyl)-2,3-dihydro-3,4-bis(2,3,4,5,6-pentafluorophenyl)-

MF C40 H8 C12 F20 N2

PAGE 1-A

PAGE 2-A

| F

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Guanidine, N-[2-[2-(pentafluorophenyl)ethenyl]phenyl]-N'-

tricyclo[3.3.1.13,7]dec-1-yl-, monohydrochloride, (E)- (9CI) MF C25 H24 F5 N3 . Cl H

Double bond geometry as shown.

● HCl

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenamine, 5-methoxy-2-[(1E)-2-(3,4,5-trifluorophenyl)ethenyl]-

MF C15 H12 F3 N O

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,1'-(1,2-ethenediyl)bis[4-[2-(pentafluorophenyl)ethenyl]- (9CI)

MF C30 H14 F10

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 9,10-Anthracenedione, 2-[2-(2,3,4,5,6-pentafluorophenyl)-2-phenylethenyl]-

MF C28 H13 F5 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, [2-(2,4-dichlorophenyl)ethenyl]pentafluoro-, (E)- (9CI)

MF C14 H5 C12 F5

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzoic acid, 4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-, methyl ester

MF C16 H9 F5 O2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3,4,5-pentafluoro-6-(2-phenyl-1-propen-1-yl)-

MF C15 H9 F5

$$\begin{array}{c|c} F & Ph \\ \hline CH & C-Me \\ \hline F & F \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,1'-[1,2-bis(4-methylphenyl)-1,2-ethenediyl]bis[2,3,4,5,6pentafluoro-

MF C28 H14 F10

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,1'-(1,2-dichloro-1,2-ethenediy1)bis[2,3,4,5,6-pentafluoro-

MF C14 C12 F10

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Acetamide, N-[(2S,11aS)-2,3,5,10,11,11a-hexahydro-5,11-dioxo-7-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-1H-pyrrolo[2,1-c][1,4]benzodiazepin-2-yl]-2-methoxy-

MF C23 H18 F5 N3 O4

Absolute stereochemistry. Double bond geometry unknown.

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3-trifluoro-5-[(1E)-2-(4-methylphenyl)ethenyl]-

MF C15 H11 F3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,1'-[1,2-bis(trifluoromethyl)-1,2-ethenediyl]bis[2,3,4,5,6-pentafluoro-, (E)- (9CI)

MF C16 F16

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,1'-(1,2-ethenediyl)bis[2,3,4,5,6-pentafluoro-

MF C14 H2 F10

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Benzeneacetonitrile, $\alpha, \alpha'-[[4,4''-bis(dimethylamino)[1,1':4',1''-terphenyl]-2',5'-diyl]dimethylidyne]bis[2,3,4,5,6-pentafluoro-, <math>(\alpha Z, \alpha' Z)-(9CI)$ MF C40 H24 F10 N4

L4201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

ΙN Benzene, 1-[2-(2,5-dimethoxyphenyl)]-2,3,4,5,6-pentafluoro-

MFC16 H11 F5 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

Benzeneacetonitrile, α -[[4-(cyanomethyl)-2,3,5,6-ΙN tetrafluorophenyl](2,3,4,5,6-pentafluorophenyl)methylene]-2,3,4,5,6pentafluoro-, compd. with N-ethylethanamine (1:1) C23 H2 F14 N2 . C4 H11 N

MF

CM 1

CM 2

H₃C-CH₂-NH-CH₂-CH₃

L4

201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN Benzeneacetonitrile, 2,3,4,5,6-pentafluoro- $\!\alpha\!-\!$ ΙN

[[(methylsulfonyl)oxy][2-(trifluoromethyl)phenyl]methylene]-

MF C17 H7 F8 N O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN L4

Benzene, 5-[(1E)-2-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-INmethoxyphenyl]ethenyl]-1,2,3-trifluoro-

C21 H25 F3 O2 Si MF

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,4,5-tetrafluoro-3,6-bis(2-phenylethenyl)-, (E,E)-, polymer with (E,E)-1,4-bis[2-(pentafluorophenyl)ethenyl]benzene (9CI)

MF (C22 H14 F4 . C22 H8 F10)x

CI PMS

CM 1

Double bond geometry as shown.

CM 2

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,4-bis[(1E)-2-(pentafluorophenyl)ethenyl]- (9CI)

MF C22 H8 F10

CI COM

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3-trifluoro-5-[(1E)-2-(4-methoxy-3-nitrophenyl)ethenyl]-MF C15 H10 F3 N O3

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Pyrrole, 2-[(Z)-[5-[(1E)-1,2-bis(2,3,4,5,6-pentafluorophenyl)ethenyl]-

2H-pyrrol-2-ylidene](2,3,4,5,6-pentafluorophenyl)methyl]-

MF C29 H7 F15 N2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 9H-Thioxanthen-9-one, 2-[2-(2,3,4,5,6-pentafluorophenyl)-1-propen-1-yl]-,

10,10-dioxide

MF C22 H11 F5 O3 S

$$\begin{array}{c|c} O & \text{Me} & F \\ \hline CH & C & F \\ \hline \\ O & O & F \end{array}$$

201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN L4

IN Benzene, [(1E)-2-(2-chlorophenyl)ethenyl]pentafluoro- (9CI) C14 H6 C1 F5 MF

Double bond geometry as shown.

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REGISTRY COPYRIGHT 2009 ACS on STN 201 ANSWERS L4

Bicyclo[2.2.2]octane, 1-propyl-4-[(1E)-2-[4-[(1E)-2-(3,4,5-ΙN trifluorophenyl)ethenyl]phenyl]ethenyl]-

MFC27 H29 F3

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenamine, N, N-dimethyl-4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-MFC16 H12 F5 N

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzoic acid, 3,3'-[(pentafluorophenyl)ethenylidene]bis[5-chloro-6-methoxy, dimethyl ester (9CI)

MF C26 H17 C12 F5 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, pentafluoro[(1E)-2-(4-nitrophenyl)ethenyl]- (9CI)

MF C14 H6 F5 N O2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Acetamide, N-[(2S,11aS)-2,3,5,10,11,11a-hexahydro-5,11-dioxo-7-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-1H-pyrrolo[2,1-c][1,4]benzodiazepin-2-yl]-2-(methylthio)-

MF C23 H18 F5 N3 O3 S

Absolute stereochemistry. Double bond geometry unknown.

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,4-bis[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-

MF C22 H8 F10

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3-trifluoro-5-[2-(4-methoxyphenyl)ethenyl]-

MF C15 H11 F3 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-phenylethenyl]-

MF C14 H7 F5

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzamide, 4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-N-[3-(phosphonooxy)propyl]-

MF C18 H15 F5 N O5 P

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,4-difluoro-2,5-bis[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-

MF C22 H6 F12

201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN L4

Benzeneacetonitrile, α -[[4-(cyanomethyl)-2,3,5,6-ΙN $\texttt{tetrafluorophenyl}] (2, 3, 4, 5, 6-\texttt{pentafluorophenyl}) \, \texttt{methylene}] \, -2, 3, 4, 5, 6-\texttt{pentafluorophenyl}) \, +2, 6-\texttt{pentafluor$ pentafluoro-, compd. with 1-butanamine (1:1) C23 H2 F14 N2 . C4 H11 N

MF

СМ 1

СМ 2

H3C-CH2-CH2-CH2-NH2

L4201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

ΙN Benzene, 1-ethyl-3, 4, 5-trifluoro-2-[(1E)-2-(3,4,5-trifluorophenyl)ethenyl]-

MF C16 H10 F6

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Phenol, 2-methoxy-5-[(1Z)-2-(3,4,5-trifluorophenyl)ethenyl]-MF C15 H11 F3 O2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzene, 1,2,4,5-tetrafluoro-3,6-bis(2-phenylethenyl)-, stereoisomer, compd. with (E,E)-1,4-bis[2-(pentafluorophenyl)ethenyl]benzene (1:1) (9CI)
MF C22 H14 F4 . C22 H8 F10

CM 1

Double bond geometry as shown.

CM 2

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,1'-(1,2-ethenediyl)bis[2,3,4,5-tetrafluoro-6[(methylthio)methyl]-

MF C18 H12 F8 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3-trifluoro-5-[(1E)-2-(4-methoxy-2-nitrophenyl)ethenyl]-

MF C15 H10 F3 N O3

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenamine, 4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-N,N-diphenyl-

MF C26 H16 F5 N

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Cinnoline, 8-[1,2-bis(pentafluorophenyl)ethenyl]-2,3-dihydro-6-methyl-2-(4-methylphenyl)-3,4-bis(pentafluorophenyl)-, (E)- (9CI)

MF C42 H14 F20 N2

| F

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,1',1'',1'''-(1,3-butadiene-1,2,3,4-tetrayl)tetrakis[2,3,4,5,6pentafluoro-

MF C28 H2 F20

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Bicyclo[2.2.2]octan-1-ol, 4-[(1E)-2-[4-[(1E)-2-(3,4,5-trifluorophenyl)]]ethenyl]ethenyl]-

MF C24 H23 F3 O

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Benzene, 1,1'-(1E)-1,2-ethenediylbis[4-[(1E)-2-(pentafluorophenyl)ethenyl]-(9CI)

MF C30 H14 F10

201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN L4

201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN Benzoic acid, 3,3'-[(pentafluorophenyl)ethenylidene]bis[5-chloro-6-methoxy-ΙN , diammonium salt (9CI)

MF C24 H13 C12 F5 O6 . 2 H3 N

$$\begin{array}{c|c} \text{OMe} & \text{CO}_2\text{H} \\ \hline \text{Cl} & \text{CO}_2\text{H} \\ \hline \text{MeO} & \text{F} & \text{F} \\ \hline \text{CO}_2\text{H} & \text{F} \end{array}$$

●2 NH3

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Benzenemethanol, α -[(2,3,4,5,6-pentafluorophenyl)methylene]-, sodium ΙN salt (1:1)

C14 H7 F5 O . Na MF

Na

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Benzenediol, 5-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-2-propyl-

MF C17 H13 F5 O2

$$\begin{array}{c|c} F & \text{OH} \\ \hline F & F & \text{OH} \\ \hline \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1-[(1E)-2-[4-(1,1-dimethylethyl)phenyl]ethenyl]-2,5-difluoro-4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-

MF C26 H19 F7

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3,4,5-pentafluoro-6-[2-(4-methoxyphenyl)ethenyl]-

MF C15 H9 F5 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,1'-(1E)-1,2-ethenediylbis[2,3,4,5,6-pentafluoro-

MF C14 H2 F10

CI COM

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenamine, N,N-dimethyl-4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)-1-propen-1-y1]-

MF C17 H14 F5 N

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetaldehyde, α -[(1,3-dihydro-1,3,3-trimethylspiro[2H-indole-2,3'-[3H]naphth[2,1-b][1,4]oxazin]-5'-yl)methylene]-2,3,4,5,6-pentafluoro-MF C31 H21 F5 N2 O2

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetonitrile, α -[[4-(cyanomethyl)-2,3,5,6-tetrafluorophenyl](2,3,4,5,6-pentafluorophenyl)methylene]-2,3,4,5,6-pentafluoro-

MF C23 H2 F14 N2

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1-[(1E)-1,2-diphenylethenyl]-2,3,4,5,6-pentafluoro-

MF C20 H11 F5

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzene, 1,2,3-trifluoro-5-[(1Z)-2-(3-fluoro-4-methoxyphenyl)ethenyl]MF C15 H10 F4 O

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzene, 1,1',1'',1'''-methanetetrayltetrakis[4-[2-(pentafluorophenyl)ethenyl]-, (all-E)- (9CI)
MF C57 H24 F20

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 1,3-Benzodioxole, 5-[2-(pentafluorophenyl)ethenyl]-, (Z)- (9CI) MF C15 H7 F5 O2

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Pyridinium, 1-[(1Z)-1-cyano-2-[2-[(1Z)-1-cyano-2-phenylethenyl]-3,4,5,6-tetrafluorophenyl]-2-hydroxyethenyl]-, inner salt

MF C23 H11 F4 N3 O

Double bond geometry as shown.

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,1'-[1-[(4-methylphenyl)sulfonyl]-1,2-ethenediyl]bis[2,3,4,5,6pentafluoro- (9CI)

MF C21 H8 F10 O2 S

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenamine, N-methyl-4-[2-(2,3,4,5-tetrafluoro-6-nitrophenyl)ethenyl]-N-

[2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl]-

MF C22 H22 F4 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3,4,5-pentafluoro-6-[(1Z)-2-phenylethenyl]-

MF C14 H7 F5

Double bond geometry as shown.

$$\begin{matrix} F & & & \\ & & & \\ F & & & \\ F & & \end{matrix} Ph$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1, 2, 3, 4, 5-pentafluoro-6-[(1E)-2-(3, 4, 5-trimethoxyphenyl)ethenyl]-

MF C17 H13 F5 O3

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzene, 1,1'-(1Z)-1,2-ethenediylbis[3,4,5-trifluoro- (9CI)

MF C14 H6 F6

Double bond geometry as shown.

$$\begin{array}{c|c} F & & F \\ \hline F & & F \\ \hline \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzene, 1,2,3,4-tetrafluoro-5-[2-(4-methoxyphenyl)ethenyl]-, (E)- (9CI)
MF C15 H10 F4 O

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Acrylonitrile, 2,3-bis(pentafluorophenyl)-, (Z)- (8CI) MF C15 H F10 N

Double bond geometry as shown.

$$\begin{array}{c|c} F & F \\ \hline F & CN \\ \hline F & F \\ \hline \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1-[2-[4-[2-[4-[2-(4-methoxyphenyl)ethenyl]phenyl]ethenyl]-2,5-dipropylphenyl]ethenyl]phenyl]ethenyl]-4-[2-[4-[2-[4-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-2,5-dipropylphenyl]ethenyl]phenyl]ethenyl]-2,5-dipropyl-

MF C81 H81 F5 O

PAGE 1-C

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Butenedinitrile, 2,3-bis(pentafluorophenyl)-, radical ion(1-), vanadium(2+), (2E)- (9CI)

MF C16 F10 N2 . 1/2 V

CI COM, RIS

●1/2 V(II) 2+

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenamine, N-[4-(2,2-diphenylethenyl)phenyl]-2,4,6-trimethyl-N-[4-[2-(2,3,4,5,6-pentafluorophenyl)-2-phenylethenyl]phenyl]-

MF C49 H36 F5 N

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Stilbene, α -chloroundecafluoro- (7CI, 8CI)

MF C14 Cl F11

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Benzenediol, 2-(1-methylethyl)-5-[2-(2,3,4,5,6-

pentafluorophenyl)ethenyl]-

MF C17 H13 F5 O2

$$\begin{array}{c|c} F & \text{OH} \\ \hline F & \text{F} & \text{OH} \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Diazene, 1-[2,6-bis[(1Z)-1,2-bis(2,3,4,5,6-pentafluorophenyl)ethenyl]-3,5-dichlorophenyl]-2-phenyl-, (1E)-

MF C40 H8 Cl2 F20 N2

Double bond geometry as shown.

PAGE 1-A

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MF C30 H6 F18

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α -[(2,3,4,5,6-pentafluorophenyl)methylene]-

MF C15 H7 F5 O2

$$\begin{array}{c|c} F & Ph \\ \hline \\ F & CH = C-CO_2H \end{array}$$

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzonitrile, 4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-

MF C15 H6 F5 N

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1-[trans-4-[4-(4-propylphenyl)butyl]cyclohexyl]-4-[2-(3,4,5-trifluorophenyl)ethenyl]-

MF C33 H37 F3

Relative stereochemistry.

Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, pentafluoro[2-(4-methoxyphenyl)ethenyl]-, (Z)- (9CI)

MF C15 H9 F5 O

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzoic acid, 4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)]- MF C15 H7 F5 O2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzonitrile, 2,3,5,6-tetrafluoro-4-[2-(2,3,4,5,6-

pentafluorophenyl)ethenyl]MF C15 H2 F9 N

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,1'-[1,2-bis(phenylmethylene)-1,2-ethanediyl]bis[2,3,4,5,6-pentafluoro-(9CI)

MF C28 H12 F10

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1-[(1E)-2-(3-chlorophenyl)-1-(4-methylphenyl)-1-buten-1-yl]-2,3,4,5,6-pentafluoro-

MF C23 H16 C1 F5

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3-trifluoro-5-[(1Z)-2-(3,4,5-trimethylphenyl)ethenyl]-MF C17 H15 F3

MF C1/ 1113 F3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetonitrile, α -[[3-(cyclopentyloxy)-4-methoxyphenyl]methylene]-2,3,4,5,6-pentafluoro-, (Z)- (9CI)

MF C21 H16 F5 N O2

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, 2,3,4,5,6-pentafluoro- α -[(2,3,4,5,6-pentafluorophenyl)methylene]-

MF C15 H2 F10 O2

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetonitrile, 3,4-dimethoxy- α -[(3,4,5-trifluorophenyl)methylene]-, (α Z)-

MF C17 H12 F3 N O2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Poly[[1,1'-biphenyl]-4,4'-diyl[(1E)-1,2-bis(pentafluorophenyl)-1,2ethenediyl]] (9CI)

MF (C26 H8 F10)n

CI PMS

PAGE 2-A

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Benzeneacetonitrile, α -[[4-(cyanomethy1)-2,3,5,6-ΙN tetrafluorophenyl](2,3,4,5,6-pentafluorophenyl)methylene]-2,3,4,5,6-pentafluoro-, compd. with N-butyl-1-butanamine (1:1) C23 H2 F14 N2 . C8 H19 N

MF

CM1

CM 2

n-Bu-NH-Bu-n

L4

201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN 2-Propenoic acid, 3-[5-[4-[2,2-bis(2,3,4,5,6-ΙN

pentafluorophenyl)ethenyl]phenyl]-2-thienyl]-2-cyano-, (2Z)-

MF C28 H9 F10 N O2 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2009 ACS on STN L4

ΙN Benzeneacetic acid, 4-methoxy- α -[(3,4,5-trifluorophenyl)methylene]-, $(\alpha E) -$

MF C16 H11 F3 O3

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Diazene, 1-[2-[(1E)-1,2-bis(2,3,4,5,6-pentafluorophenyl)ethenyl]-3,5-dichlorophenyl]-2-phenyl-, (1E)-

MF C26 H8 C12 F10 N2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Imidazole, 4,4'-[1,2-bis(pentafluorophenyl)-1,2-ethenediyl]bis[2,5-dihydro-1,2,2,5,5-pentamethyl-, 3,3'-dioxide (9CI)

MF C30 H30 F10 N4 O2

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzenamine, 2-methoxy-5-[(1Z)-2-(3,4,5-trifluorophenyl)ethenyl]MF C15 H12 F3 N O

Double bond geometry as shown.

$$\begin{array}{c|c} F & & Z \\ \hline F & & NH_2 \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-(2-nitrophenyl)ethenyl]MF C14 H6 F5 N O2

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 9,10-Anthracenedione, 2-[2,2-bis(2,3,4,5,6-pentafluorophenyl)ethenyl]-7-(1,1-dimethylethyl)-

MF C32 H16 F10 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1-[(1E)-2-(4-bromophenyl)ethenyl]-2,3,4,5,6-pentafluoro-

MF C14 H6 Br F5

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzene, 5-[(1Z)-1-(chloromethyl)-2-(4-fluorophenyl)ethenyl]-1,2,3-trifluoro-

MF C15 H9 Cl F4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[(1E)-2-(2,3,4,5,6pentafluorophenyl)ethenyl]-, (4S,4aS,5aR,12aS)MF C29 H23 F5 N2 O7

Absolute stereochemistry. Double bond geometry as shown.

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3,4-tetrafluoro-5-[2-[4-(4-pentylcyclohexyl)phenyl]ethenyl]-, [1 α (E),4 β]- (9CI)

MF C25 H28 F4

Relative stereochemistry.
Double bond geometry as shown.

Me (CH₂)
$$\frac{F}{4}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Titanium, [1,2-bis(pentafluorophenyl)-1-propenyl]bis(η 5-2,4-cyclopentadien-1-yl)methyl- (9CI)

MF C26 H16 F10 Ti

CI CCS

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Acetamide, N-[(2S,11aS)-2,3,5,10,11,11a-hexahydro-5,11-dioxo-7-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-1H-pyrrolo[2,1-c][1,4]benzodiazepin-

2-y1]-MF C22 H16 F5 N3 O3

Absolute stereochemistry.

Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1, 2, 3-trifluoro-5-[(1Z)-2-(4-methylphenyl)ethenyl]-

MF C15 H11 F3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,1'-[1,2-bis(trifluoromethy1)-1,2-ethenediy1]bis[2,3,4,5,6pentafluoro-, (Z)- (9CI)

MF C16 F16

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Acrylic acid, 2-(pentafluorophenyl)-3-phenyl-, compd. with 2-benzyl-2-thiopseudourea (1:1), (E)- (8CI)

MF C15 H7 F5 O2 . C8 H10 N2 S

CM 1

Double bond geometry as shown.

CM 2

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Naphthacenecarboxamide, 1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-, (4aS,5aR,12aS)-

MF C27 H18 F5 N O7

Absolute stereochemistry. Double bond geometry unknown.

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3,4,5-pentafluoro-6-[2-(3,4,5-trimethoxyphenyl)ethenyl]-

MF C17 H13 F5 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetonitrile, $\alpha-[[4-(\text{cyanomethy1})-2,3,5,6-\text{tetrafluoropheny1}](2,3,4,5,6-\text{pentafluoropheny1}) methylene]-2,3,4,5,6-pentafluoro-, compd. with N-propyl-1-propanamine (1:1)$

MF C23 H2 F14 N2 . C6 H15 N

CM 1

CM 2

n-Pr-NH-Pr-n

L4

201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN Benzeneacetonitrile, 2,3,4,5,6-pentafluoro- $\alpha\text{-}[\text{hydroxy}[2\text{-}$ ΙN (trifluoromethyl)phenyl]methylene]-

MF C16 H5 F8 N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN L4

Phenol, 2-methoxy-5-[(1E)-2-(3,4,5-trifluorophenyl)ethenyl]-ΙN

MF C15 H11 F3 O2

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,1'-Biphenyl, 4,4'-bis[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-

MF C28 H12 F10

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Guanidine, N-[2-[2-(pentafluorophenyl)ethenyl]-N'-tricyclo[3.3.1.13,7]dec-1-yl-, (E)- (9CI)

MF C25 H24 F5 N3

CI COM

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenamine, 5-methoxy-2-[(1Z)-2-(3,4,5-trifluorophenyl)ethenyl]-

MF C15 H12 F3 N O

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenamine, N, N-dimethyl-4-[(1Z)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-

MF C16 H12 F5 N

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 9H-Thioxanthen-9-one, 6-(1,1-dimethylethyl)-2-[2-(2,3,4,5,6-

pentafluorophenyl)-2-phenylethenyl]-, 10,10-dioxide

MF C31 H21 F5 O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, pentafluoro[2-(4-fluorophenyl)ethenyl]-, (E)- (9CI)

MF C14 H6 F6

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Propenoic acid, 2-methyl-, 11-[4-[(1E)-2-cyano-2-(2,3,4,5,6-pentafluorophenyl)] ethenyl]-2-methoxyphenoxy]undecyl ester

MF C31 H34 F5 N O4

F CN
$$E$$
 E F F CH_2 CH_2

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3,4,5-pentafluoro-6-(2-phenylethenyl)-

MF C14 H7 F5

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 5-[1,2-difluoro-2-(4-pentylphenyl)ethenyl]-1,2,3-trifluoro-, (Z)-(9CI)

MF C19 H17 F5

$$F$$
 Z
 F
 F
 C
 $CH_2)_4$
 Me

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, [(1E)-2-(4-chlorophenyl)ethenyl]pentafluoro- (9CI)

MF C14 H6 C1 F5

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Urea, N-[(2S,11aS)-2,3,5,10,11,11a-hexahydro-5,11-dioxo-7-[2-(2,3,4,5,6pentafluorophenyl)ethenyl]-1H-pyrrolo[2,1-c][1,4]benzodiazepin-2-yl]-N'-(1methylethyl)-

MF C24 H21 F5 N4 O3

Absolute stereochemistry. Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,4-difluoro-2,5-bis[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-

MF C22 H6 F12

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzene, 1,1'-(1,2-ethenediyl)bis[2,3,4,5-tetrafluoro-, (Z)- (9CI) MF C14 H4 F8

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Acrylic acid, 2-(pentafluorophenyl)-3-phenyl-, (E)- (8CI) MF C15 H7 F5 O2

CI COM

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

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COST IN U.S. DOLLARS

SESSION ENTRY 194.04 FULL ESTIMATED COST 194.48

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=> s 14

L5 152 L4

=> d ibib abs hitstr 150-152

ANSWER 150 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

1967:500075 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 67:100075

ORIGINAL REFERENCE NO.: 67:18823a, 18826a

Reaction of pentafluorobenzonitrile with hydroxylamine TITLE: AUTHOR(S): Shchegoleva, G. S.; Barkhash, V. A.; Vorozhtsov, N.

N., Jr.

CORPORATE SOURCE: Novosibirsk Inst. Organ. Khim., Novosibirsk, USSR SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya

(1967), (3), 708-9 CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE: Journal LANGUAGE: Russian

For diagram(s), see printed CA Issue. GT

cf. CA 64: 12586d. To 1 g. C6F5CN and 1.4 g. HONH2.HCl in EtOH at AR 0° was added slowly 0.8 g. Na2CO3 in H2O, the mixture kept 6 hrs. at

 0° , extracted with Et20, and the evaporated extract treated with 24% HBr gave

64% 2,3,4,5,6-pentafluorobenzamidoxime-HBr, m. 193-6°; free oxime (I) m. 94-7° (after sublimation). I (0.5 g.) and 1.5 g. C6F5COC1 heated 0.5 hr. in C6H6 gave 80% C6F5C(NH2):NO2CC6F5 (II), m. 147-51°. BzCl similarly gave the benzoate, m. 160-5°. Refluxing II with POCl3 3 hrs. gave, after treatment with ice, 96% 3,5-bis(pentafluorophenyl)-1,2,4-oxadiazole (III), m. 100-1°. Similarly was prepared 3-pentafluorophenyl-5-phenyl-1,2,4-oxadiazole (IV), m. 88-93°. Ir spectra are reported, along with N.M.R. spectra, which confirmed the above structures.

IT 1081539-80-1P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation) (Reaction of pentafluorobenzonitrile with hydroxylamine)

RN 1081539-80-1 CAPLUS

CN Benzenemethanamine, 2,3,4,5,6-pentafluoro- α -[nitro(2,3,4,5,6-pentafluorophenyl)methylene]- (CA INDEX NAME)

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L5 ANSWER 151 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1967:421520 CAPLUS

DOCUMENT NUMBER: 67:21520

ORIGINAL REFERENCE NO.: 67:4055a,4058a

TITLE: Polyfluoroarenes. IX. Decafluorotolan: synthesis,

properties, and use as an organometallic ligand

AUTHOR(S): Birchall, John M.; Bowden, F. L.; Haszeldine, Robert

N.; Lever, Alfred B. P.

CORPORATE SOURCE: Univ. Manchester, Manchester, UK

SOURCE: Journal of the Chemical Society [Section] A:

Inorganic, Physical, Theoretical (1967), (5), 747-53

CODEN: JCSIAP; ISSN: 0022-4944

DOCUMENT TYPE: Journal LANGUAGE: English

AB cf. CA 66: 37126j. IC.tplbond.CI and C6F5MgBr give decafluorotolan (C6F5C.tplbond.CC6F5) in good yield. The triple bond in the tolan undergoes ready catalytic hydrogenation, addition of Br, and oxidative cleavage, but is relatively unreactive towards hydration, iodination, and carbonylation. Decafluorotolan reacts with methoxide ion in the 4- and 4'-positions, and gives a good yield of

tetrakis(pentafluorophenyl)thiophene when it is heated with S. Reaction of the tolan with Co octacarbonyl yields a complex

Co2(CO)6(C6F5C.tplbond.CC6F5), shown by its chemical and spectroscopic properties to be similar in structure to its hydrocarbon analog; octafluoro-4,4'-dimethoxytolan behaves similarly.

Tetrakis(pentafluorophenyl)cyclopentadienone (perfluorotetracyclone) is obtained when a solution of the Co carbonyl complex of decafluorotolan is heated. Reaction of decafluorotolan with Fe penta- or dodecacarbonyl yields a complex Fe2(CO)6(C6F5C.tplbond.CC6F5)2, together with perfluorotetracyclone. 21 references.

IT 14992-38-2P 14992-40-6P 14992-41-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
RN 14992-38-2 CAPLUS
CN Benzene, 1,1'-(1Z)-1,2-ethenediylbis[2,3,4,5,6-pentafluoro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 14992-40-6 CAPLUS

CN Benzene, 1,1'-(1E)-1,2-ethenediylbis[2,3,4,5,6-pentafluoro- (CA INDEX NAME)

Double bond geometry as shown.

RN 14992-41-7 CAPLUS

CN Benzene, 1,1'-(1,2-dibromo-1,2-ethenediyl)bis[2,3,4,5,6-pentafluoro- (CA INDEX NAME)

OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

L5 ANSWER 152 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1966:67439 CAPLUS

DOCUMENT NUMBER: 64:67439
ORIGINAL REFERENCE NO.: 64:12576a-c

TITLE: Aromatic polyfluoro compounds. XXVIII. Further

reactions of the pentafluorophenyl anion

AUTHOR(S): Callander, D. D.; Coe, P. L.; Tatlow, J. C.

CORPORATE SOURCE: Univ. Birmingham, UK

SOURCE: Tetrahedron (1966), 22(2), 419-32 CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: English

AB cf. CA 64, 1987f. The pentafluorophenyl anion from

pentafluorophenyllithium was used as a nucleophile and as a source of tetrafluorobenzyne. As a nucleophile, it was used to make polyfluorobiand -terphenyl derivs. from perfluorotoluene, perfluoro-o-xylene,

pentafluoronitrobenzene and bromopentafluorobenzene, and polyfluoropolyaryls from perfluorobiphenyl. It also attacked decafluorocyclohexene and chlorotrifluoroethylene, presumably by an addition-elimination sequence. Reactions using the tetrafluorobenzene

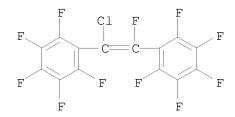
addition-elimination sequence. Reactions using the tetrafluorobenzyne intermediate were carried out in the presence of excess

bromopentafluorobenzene, pentafluorobenzene, and various lithium halides, in some cases with variation of the solvent. A mechanism for some of these reactions is postulated.

IT 5576-21-6P, Stilbene, α -chloroundecafluoro-

RN 5576-21-6 CAPLUS

CN Stilbene, α -chloroundecafluoro- (7CI, 8CI) (CA INDEX NAME)



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)

=> d ibib abs hitstr 140-149

L5 ANSWER 140 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1973:546162 CAPLUS

DOCUMENT NUMBER: 79:146162

ORIGINAL REFERENCE NO.: 79:23689a,23692a

TITLE: Decafluoro- α , β -dichlorostilbene

INVENTOR(S): Dvornikova, K. V.; Platonov, V. E.; Yakobson, G. G.

PATENT ASSIGNEE(S): Novosibirsk Institute of Organic Chemistry

SOURCE: U.S.S.R. From: Otkrytiya, Izobret., Prom. Obraztsy,

Tovarnye Znaki 1973, 50(32), 49.

CODEN: URXXAF

DOCUMENT TYPE: Patent LANGUAGE: Russian

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 392060	A1	19730727	SU 1971-1690000	19710804
PRIORITY APPLN. INFO.:			SU 1971-1690000 A	19710804
AB (C6F5CCl:)2 was prej	pared b	y heating	C6F5CCl3 in the presence	of Cu at
400-500° or at 150-3	200° in	a closed	system.	

49763-76-0P ΤТ

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

49763-76-0 CAPLUS RN

Benzene, 1,1'-(1,2-dichloro-1,2-ethenediyl)bis[2,3,4,5,6-pentafluoro- (CA CN INDEX NAME)

ANSWER 141 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1972:501784 CAPLUS

DOCUMENT NUMBER: 77:101784

ORIGINAL REFERENCE NO.: 77:16783a,16786a

TITLE: Reaction of phosphorus ylides with perfluorobenzene AUTHOR(S): Nesmeyanov, N. A.; Berman, S. T.; Reutov, O. A. Mosk. Gos. Univ. im. Lomonosova, Moscow, USSR CORPORATE SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya SOURCE:

(1972), (3), 605-6

CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE: Journal LANGUAGE: Russian

AΒ Under argon, MePh3PI and PhLi in Et2O-C6H6, kept 2.5 hr, filtered and treated with C6F6 2 hr, gave Ph3P:C(C6F5)H which was treated in situ with p-O2NC6H4CHO 12 hr to give 62% trans-C6F5CH:CHC6-H4NO2-p. Similarly formed was the p-Cl analog (51%). Ph2P(CH2Ph)Cl treated with BuLi in THF-Et20 gave the corresponding ylide in solution, which was treated with C6F6 to give a solution of Ph3P+CH(C6F5)Ph F- (I). I reacted with the residual ylide to form Ph3P:CPhC6F5 (II) in solution along with Ph3P+CH2Ph F-. Treated with aqueous NH4BF4, this gave PhCH2P+Ph3-BF4 while the organic phase gave 85% II. II with dry HCl formed the conjugate acid, which reverted to the ylide on contact with a nucleophile, e.g., aqueous Na2CO3. ΙT 37516-14-6P 37516-15-7P

(preparation of)

RN 37516-14-6 CAPLUS

Benzene, pentafluoro[(1E)-2-(4-nitrophenyl)ethenyl]- (9CI) (CA INDEX CN NAME)

RL: SPN (Synthetic preparation); PREP (Preparation)

RN 37516-15-7 CAPLUS

CN Benzene, [(1E)-2-(4-chlorophenyl)ethenyl]pentafluoro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L5 ANSWER 142 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1971:469273 CAPLUS

DOCUMENT NUMBER: 75:69273

ORIGINAL REFERENCE NO.: 75:10951a,10954a

TITLE: Aromatic fluorinated derivatives. XLIII. Equilibrium

acidity of pentafluorophenyl methanes

AUTHOR(S): Vlasov, V. M.; Krivousova, E. D.; Yakobson, G. G. CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, USSR Zhurnal Organicheskoi Khimii (1971), 7(5), 986-9

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal LANGUAGE: Russian

The reaction of NaH with C6F5CH2COPh (I) in MeOCH2CH2OMe solution gives C6F5CH:CPhO-Na+ (II). Similarly, C6F5CH:C(C6Cf5)O-Na+ (III) is obtained. NMR spectra of p- and m- F atoms of II and III show more pos. chemical shifts than the spectra of I or C6F5CH2COC6F5 (IV). PK values of I and IV are resp. 15.3 and 11.7. This pK shift, which is due to the replacement of Ph with C6F5, is considerably greater than expected because of the relatively small contribution of resonance towards the stabilization of II or III carbanions.

IT 33753-91-2 33753-92-3

RL: PRP (Properties)

(nuclear magnetic resonance of)

RN 33753-91-2 CAPLUS

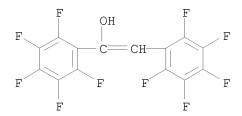
CN Benzenemethanol, α -[(2,3,4,5,6-pentafluorophenyl)methylene]-, sodium salt (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} F & Ph \\ \hline CH = C - OH \\ \hline F & F \end{array}$$

Na

RN 33753-92-3 CAPLUS

CN Benzenemethanol, 2,3,4,5,6-pentafluoro- α -[(2,3,4,5,6-pentafluorophenyl)methylene]-, sodium salt (1:1) (CA INDEX NAME)



Na

L5 ANSWER 143 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1970:31402 CAPLUS

DOCUMENT NUMBER: 72:31402

ORIGINAL REFERENCE NO.: 72:5717a,5720a

TITLE: Aromatic fluoro-derivatives. XXXVII. Reaction of

pentafluorophenylacetonitrile with aldehydes in the

presence of potassium fluoride

AUTHOR(S): Vlasov, V. M.; Yakobson, G. G.

CORPORATE SOURCE: Novosibirsk. Inst. Org. Khim., Novosibirsk, USSR

SOURCE: Zhurnal Obshchei Khimii (1969), 39(9), 2071-5

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal LANGUAGE: Russian

AB C6F5CH2CN (I) and paraformaldehyde kept 7 hr in (CH2OMe)2 in the presence

of KF gave 42% C6F5CH(CN)CH2OH ("pentafluoroatroponitrile"), b0 \cdot 2

 $110-12^{\circ}$, m. $41.5-2.5^{\circ}$, and 22% CH2[CH(CN)C6F5]2, m.

100-11°, both characterized by NMR and ir spectra. Similar

reaction but with C6F5CHO in the presence of KF converted I into 17% cis-decafluorocyanostilbene, m. $103-5^{\circ}$, its mixture with the trans

isomer (2%), m. $85-95^{\circ}$; and 8%

1,2-bis(pentafluorophenyl)-2-cyanoethanol, m. 146-8.5°; all were

characterized by NMR spectra; the residue gave some C6F5CH2CONH2, m. $178-81.5^{\circ}$. Thus KF catalyzes condensations of I with aldehydes.

IT 25529-43-5P 25576-30-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 25529-43-5 CAPLUS

CN Acrylonitrile, 2,3-bis(pentafluorophenyl)-, (E)- (8CI) (CA INDEX NAME)

RN 25576-30-1 CAPLUS

CN Acrylonitrile, 2,3-bis(pentafluorophenyl)-, (Z)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.

L5 ANSWER 144 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1969:524121 CAPLUS

DOCUMENT NUMBER: 71:124121

ORIGINAL REFERENCE NO.: 71:23055a,23058a

TITLE: Transformations of decafluoro- α -phenylcinnamic

acid

AUTHOR(S): Molosnova, V. P.; Barkhash, V. A.; Vorozhtsov, N. N.,

Jr.

CORPORATE SOURCE: Novosibirsk. Inst. Org. Khim., Novosibirsk, USSR SOURCE: Zhurnal Obshchei Khimii (1969), 39(8), 1774-7

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal LANGUAGE: Russian

AB RMgCl from 20.8 g. C6F5Cl, prepared in N atmospheric was treated with dry CH2O $\,$

over

30-40 min., then treated with ice-HCl to yield 73% C6F5CH2OH, b57 113-14.5°, m. 30-1°. C6F5CH0 heated in Ac20-Et3N with C6F5CH2CO2H (prepared from above carbinol via treatment with PCl5, KCN and H2O), 0.5 hr. gave after acidification a mixture of 63.6% C6F5CH:CPhCO2H (I), m. 187-8°, and 2% 3-pentafluorophenyl-5,6,7,8-tetrafluorocoumarin, m. 210-11°. I gave the S-benzylthiuronium salt, m. 167-7.5°. I heated with KF in Me2NCHO 5 hrs. gave 3-pentafluorobenzylidene-4,5,6,7-tetrafluoro-2-coumarone, m. 185-7°, which with KMnO4 was oxidized to tetrafluorosalicylic acid, m. 169-70°. I and 20% oleum in CHCl3 at 40°, treated with NaN3, then quenched in ice, gave 73.5% decafluorodeoxybenzoin, m.

81-2°. Ir spectra were reported.

IT 1081539-52-7P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation) (Transformations of decafluoro- α -phenylcinnamic acid)

RN 1081539-52-7 CAPLUS

CN Benzeneacetic acid, $\alpha-[(2,3,4,5,6-pentafluorophenyl)methylene]-$ (CA INDEX NAME)

$$\begin{array}{c|c}
F & Ph \\
CH = C - CO_2H \\
F & F
\end{array}$$

IT 24043-87-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reactions of)

RN 24043-87-6 CAPLUS

CN Benzeneacetic acid, 2,3,4,5,6-pentafluoro- α -[(2,3,4,5,6-pentafluorophenyl)methylene]- (CA INDEX NAME)

IT 25955-31-1P

RN 25955-31-1 CAPLUS

CN Benzeneacetic acid, 2,3,4,5,6-pentafluoro- α -[(2,3,4,5,6-pentafluorophenyl)methylene]-, compd. with phenylmethyl carbamimidothioate (1:1) (CA INDEX NAME)

CM 1

CRN 24043-87-6 CMF C15 H2 F10 O2

CM 2

CRN 621-85-2 CMF C8 H10 N2 S

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD

(3 CITINGS)

L5 ANSWER 145 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1969:403064 CAPLUS

DOCUMENT NUMBER: 71:3064
ORIGINAL REFERENCE NO.: 71:556h,557a

TITLE: Transannular interactions in tetrafluoro[2.2]paracyclophane AUTHOR(S): Filler, Robert; Choe, E. W.

CORPORATE SOURCE: Illinois Inst. of Technol., Chicago, IL, USA SOURCE: Journal of the American Chemical Society (1969),

91(7), 1862-4

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

The Wittig reaction of BzH and C6F5CH:PPh3, prepared by treating C6F5CH2PPh3Br with BuLi, gave trans-C6F5CH:CHPh which was hydrogenated to C6F5CH2CH2Ph. H was introduced into the fluorinated ring and the product was converted to 4-formyl-2,3,5,6-tetrafluorobibenzyl (I) by treatment with BuLi, followed by N-methylformanilide. Reduction of I with LiAlH4 gave the alc., which was treated with PBr3. The bromide obtained was bromomethylated to give 4,4'-bis(bromomethyl)-2,3,5,6-tetrafluorobibenzyl, which was subjected to a Wurtz reaction to give 4,5,7,8-tetrafluoro[2.2]paracyclophane (II). The uv spectra of [2.2]paracyclophane, II, and octafluoro[2.2]paracyclophane were tabulated and discussed. The 1H N.M.R. spectrum of II in CC14 revealed transannular coupling between the aromatic protons of 1 ring and the F atoms of the other.

IT 19292-25-2P

RN 19292-25-2 CAPLUS

CN Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-phenylethenyl]- (CA INDEX NAME)

(6 CITINGS)

L5 ANSWER 146 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1969:106077 CAPLUS

DOCUMENT NUMBER: 70:106077

ORIGINAL REFERENCE NO.: 70:19783a,19786a

TITLE: Synthesis of cis- and trans-decafluorostilbenes
AUTHOR(S): Molosnova, V. P.; Vysochin, V. I.; Barkhash, V. A.;

Vorozhtsov, N. N., Jr.

CORPORATE SOURCE: Novosibirsk. Inst. Org. Khim., Novosibirsk, USSR SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya

(1969), (1), 146-7

CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE: Journal LANGUAGE: Russian

AB Heating 2.15 g. C6F5CH:C(C6F5)CO2Ag with 0.05 g. Cu chromite catalyst and 6.4 ml. dry Me2NCHO 4 hrs. at 160-5° gave after an aqueous treatment 49% mixed isomers of C6F5CH: CHC6F5 m. 50-60°, which after repeated crystallization from EtOH-petroleum ether gave the isomer m. 61-2°, which has the cis form. The more soluble isomer, m. 54-5°, also has the cis form on the basis of its spectra (uv and N.M.R.). On standing, both isomers lose the sharpness of m.p. and become approx. the same (m. 53-61°) after several months. However, no interconversion takes place during melting. C6F5CH2Br and Ph3P in C6H6 gave the quaternary salt, m. 237-9°, which with MeONa in tetrahydrofuran 2 days at room temperature under N, then treated with C6F5CHO 1 day at room temperature and 6 hrs. at

reflux, gave Ph3PO and 32% trans-C6F5CH:CHC6F5, m. 101.5-3.5°.

IT 14992-38-2P 14992-40-6P

RN 14992-38-2 CAPLUS

CN Benzene, 1,1'-(1Z)-1,2-ethenediylbis[2,3,4,5,6-pentafluoro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 14992-40-6 CAPLUS

CN Benzene, 1,1'-(1E)-1,2-ethenediylbis[2,3,4,5,6-pentafluoro- (CA INDEX NAME)

L5 ANSWER 147 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1969:67706 CAPLUS

DOCUMENT NUMBER: 70:67706

ORIGINAL REFERENCE NO.: 70:12629a,12632a

TITLE: Diels-Alder reactions of

polyfluorocyclohexa-1,3-dienes. I. Addition of alkynes to perfluorocyclohexa-1,3-diene. Route to

ortho-disubstituted tetrafluorobenzenes

AUTHOR(S): Anderson, Leonard Philip; Feast, William J.; Musgrave,

William K. R.

CORPORATE SOURCE: Univ. Sci. Lab., Durham City, UK

SOURCE: Journal of the Chemical Society [Section] C: Organic

(1969), (2), 211-17

CODEN: JSOOAX; ISSN: 0022-4952

DOCUMENT TYPE: Journal LANGUAGE: English

AB Perfluorocyclohexa-1,3-diene reacts with alkynes XC.tplbond.CY by

1,4-addition to give, exclusively and in good yield, 2-(X-substituted)-3-(Y-substituted)-1,4,5,6,7,7,8,8-

octafluorobicyclo[2.2.2]octa-2,5-dienes (X = Y = CF3, Me, CH2Cl, CO2Et; X

= H, Y = CF3, Me, CH2Cl, Ph; X = CF3, Y = Me) which eliminate tetrafluoroethylene on pyrolysis to give ortho-disubstituted tetrafluorobenzenes, or their further pyrolysis products

1-(X-substituted)-2-(Y-substituted)-3,4,5,6-tetrafluorobenzene (X = Y = CF3, Me, H; X = H, Y = CF3, Me, CH2C1, CO2H, C.tplbond.CH, CH:CHC6HF4, Ph;

X = CF3, Y = Me).IT 21651-69-4P

RN 21651-69-4 CAPLUS

CN Benzene, 1,1'-(1,2-ethenediyl)bis[2,3,4,5-tetrafluoro-, (E)- (9CI) (CA INDEX NAME)

OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

L5 ANSWER 148 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1968:443571 CAPLUS

DOCUMENT NUMBER: 69:43571
ORIGINAL REFERENCE NO.: 69:8147a,8150a

TITLE: Thermolysis of aromatic aldazines. IV. Similarities

and differences with electron-impact fragmentation

AUTHOR(S): Buu-Hoi, N. P.; Saaint-Ruf, Germain

CORPORATE SOURCE: Inst. Chim. Subst. Natur., C.N.R.S., Gif-Sur-Yvette,

Fr.

SOURCE: Bulletin de la Societe Chimique de France (1968), (2),

661-4

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal LANGUAGE: French

GI For diagram(s), see printed CA Issue.

The thermal decomposition of aromatic aldazines was examined by mass AB spectrometry. Thus, 5.4 g. C6D5CHO was refluxed 3 hrs. with 1.2 g. 98% N2H4.H2O and 28 ml. EtOH to give I, m. 93°. I (5 g.) was heated at 200° till gases ceased to evolve, cooled, and distilled in vacuo to give C6D5CN (II) b. 233°, III, m. 125°, and IV, m. 275°. II, on KOH saponification gave C6D5CO2H, m. 122°. C6F5CHO (5.9 g.) was refluxed 2 hrs. with 0.75 g. N2H4.H2O in 50 ml. EtOH to give 95% pentafluorobenzaldazine (V), m. 138°. V was heated 1 hr. at 280° in paraffin oil to give C6F5CH:CHC6F5 (VI), m. 101°; resolidified and remelted 158° (hexane). VI was also prepared in 50% yield by direct heating of V. The m/e, and % abundance of the fragments produced during the thermolysis of aldazines were determined The fragmentation patterns were compared with those obtained by electronic impact techniques. A bond cleavage between the aryl group and the rest of the aldazine mol. was observed during thermolysis.

IT 19339-50-5P

RN 19339-50-5 CAPLUS

CN Benzene, 1,1'-(1,2-ethenediyl)bis[2,3,4,5,6-pentafluoro- (CA INDEX NAME)

ANSWER 149 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1968:426929 CAPLUS

DOCUMENT NUMBER: 69:26929

ORIGINAL REFERENCE NO.: 69:4995a,4998a

Aromatic polyfluoro compounds. XLI. Some reaction of TITLE:

pentafluorobenzaldehyde

AUTHOR(S): Aroskar, E. V.; Brown, P. J. N.; Plevey, R. G.;

Stephens, R.

CORPORATE SOURCE: Univ. Birmingham, Birmingham, UK

SOURCE: Journal of the Chemical Society [Section] C: Organic

(1968), (13), 1569-75

CODEN: JSOOAX; ISSN: 0022-4952

DOCUMENT TYPE: Journal LANGUAGE: English

For diagram(s), see printed CA Issue.

Pentafluorobenzaldehyde was converted into a range of derivs. by reactions involving the carbonyl group, viz., a pentafluorostilbene, a pentafluorocinnamic acid (I), an azine, an oxime, and a range of acetals.

Other derivs., e.g. II, were made by reactions involving replacement of F using Me2NH, NaHS, PhSNa, and NaOMe.

19573-98-9P ΙT 19292-25-2P 19292-26-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 19292-25-2 CAPLUS

Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-phenylethenyl]- (CA INDEX NAME) CN

Double bond geometry as shown.

19292-26-3 CAPLUS RN

Acrylic acid, 2-(pentafluorophenyl)-3-phenyl-, (E)- (8CI) (CA INDEX NAME) CN

RN 19573-98-9 CAPLUS

CN Acrylic acid, 2-(pentafluorophenyl)-3-phenyl-, compd. with 2-benzyl-2-thiopseudourea (1:1), (E)- (8CI) (CA INDEX NAME)

CM 1

CRN 19292-26-3 CMF C15 H7 F5 O2

Double bond geometry as shown.

CM 2

CRN 621-85-2 CMF C8 H10 N2 S

$$\begin{array}{c} \text{NH} \\ || \\ \text{H}_2 \text{N-C-S-CH}_2 \text{-Ph} \end{array}$$

OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

=> s 15 and canceer

0 CANCEER

L6 0 L5 AND CANCEER

=> s 15 and cancer

414531 CANCER 60981 CANCERS 429588 CANCER

(CANCER OR CANCERS)

L7 3 L5 AND CANCER

=> d ibib abs tot

ANSWER 1 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN T.7

ACCESSION NUMBER: 2008:1136076 CAPLUS

DOCUMENT NUMBER: 149:533971

TITLE: Design, synthesis, biochemical, and biological

evaluation of nitrogen-containing trifluoro structural

modifications of combretastatin A-4

Hall, John J.; Sriram, Madhavi; Strecker, Tracy E.; AUTHOR(S):

> Tidmore, Justin K.; Jelinek, Christopher J.; Kumar, G. D. Kishore; Hadimani, Mallinath B.; Pettit, George R.; Chaplin, David J.; Trawick, Mary Lynn; Pinney, Kevin

CORPORATE SOURCE: Department of Chemistry and Biochemistry, Baylor

University, Waco, TX, 76798-7348, USA

Bioorganic & Medicinal Chemistry Letters (2008), SOURCE:

18(18), 5146-5149

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal English LANGUAGE:

OTHER SOURCE(S): CASREACT 149:533971

GΙ

A new trifluorinated amino-combretastatin analog, AB

Ι

(Z)-2-(4'-methoxy-3'-aminophenyl)-1-(3,4,5-trifluorophenyl)ethene (I), prepared by chemical synthesis, was found to be a potent inhibitor of tubulin

assembly (IC50 = 2.9 μM), and cytotoxic against selected human cancer cell lines. This new lead compound is among the most active

from a group of related structural modifications.

OS.CITING REF COUNT: THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD 1

(1 CITINGS)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN

2004:754412 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 141:277352

TITLE: Preparation of quinone and catechol derivatives for

the treatment of cancers and other vascular

proliferative disorders

INVENTOR(S): Chaplin, David J.; Edvardsen, Klaus; Pinney, Kevin G.;

Prezioso, Joseph Anthony; Wood, Mark

Oxigene, Inc., USA PCT Int. Appl., 101 pp. PATENT ASSIGNEE(S): SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

KIND APPLICATION NO. PATENT NO. DATE DATE _____

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WO 2004078126
                         Α2
                                20040916
                                         WO 2004-US6175
                                                                   20040301
     WO 2004078126
                         А3
                                20050811
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE,
             BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU,
             MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA,
             GN, GQ, GW, ML, MR, NE, SN, TD, TG
     AU 2004218412
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                                                                   20040301
                         Α1
     CA 2516078
                                20040916
                                            CA 2004-2516078
                         Α1
                                                                   20040301
     EP 1601348
                         A2
                                20051207
                                            EP 2004-716108
                                                                   20040301
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             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK
PRIORITY APPLN. INFO.:
                                            US 2003-450565P
                                                              P 20030228
                                            US 2003-467486P
                                                               P 20030502
                                            WO 2004-US6175
                                                                A 20040301
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OTHER SOURCE(S): CASREACT 141:277352; MARPAT 141:277352 GI

The title compound I [Ring A is optionally substituted with one to five substituents selected from alkoxy, cycloalkoxy, halo, trihaloalkyl, alkyl, allyl, alc., (substituted)amino, oxo, alkanoyl, thiol, etc.; ring B comprises at lease one structure denoted by Ra and Rb which represent an ortho-quinone (-CO-CO-), or ortho-catechol (-COH-COH-) or ortho-catechol pro-drug moiety; the remaining carbons of B ring are optionally substituted with one to five substituents selected from alkoxy, cycloalkoxy, halo, trihaloalkyl, alkyl, allyl, alc., (substituted)amino, oxo, alkanoyl, thiol, etc.; Bridge X = alkene, alkane, alkyne, amide, amine, etc.] were prepared for the treatment of solid tumor cancers and other vascular proliferative disorders. For example, compound II was prepared in a multi-step synthesis starting from 5-bromo-2-hydroxy-3-methoxybenzaldehyde. The latter showed activity with IC50s of 2.1 and 0.34 $\mu\rm M$ in the tubulin binding and MTT assays.

L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 2004:681567 CAPLUS DOCUMENT NUMBER: 141:200160

TITLE: Breast cancer resistance protein (BCRP)

inhibitor

INVENTOR(S): Yamazaki, Ryuta; Nishiyama, Yukiko; Furuta, Tomio;

Matsuzaki, Takeshi; Hatano, Hiroshi; Yoshida, Oh; Nagaoka, Masato; Aiyama, Ritsuo; Hashimoto, Shusuke;

Sugimoto, Yoshikazu

PATENT ASSIGNEE(S): Kabushiki Kaisha Yakult Honsha, Japan

SOURCE: PCT Int. Appl., 91 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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	2004																	
	2515																	
EP	1591																	
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ZA	2005	0059	88		A		2006	1227		ZA	200	05-	5988				20050	726
	20051																20050	727
	2006									US	200	05-	5440	64			20050	802
	7371				В2		2008											
	2005																20050	
	2005				Α		2005	1026									20050	
IORIT:	Y APP	LN.	INFO	.:													20030	204
										WO	200	04-	JP10	67		W	20040	203
HER SO	DURCE	(S):			MAR	PAT	141:	2001	60									

OTHER SOURCE(S): MARPAT 141:200160

Ι

AΒ

protein inhibitor which contains as an active ingredient either a diphenylacrylonitrile derivative represented by the following formula (I): (I) {wherein the eight R's are the same or different and each independently represents hydrogen, hydroxy, nitro, amino, acetylamino (-NHCOCH3), cyano (-CN), formyl (-CHO), -COOR1 (R1 is hydrogen or C1-4 alkyl), -O(CH2)nCOOR2 (n is 1 to 7 and R2 is hydrogen or C1-4 alkyl), -OOCH2CH2COOR3 (R3 is hydrogen, C1-4 alkyl, (Z)-2-(3,4-dimethoxyphenyl)-3-(4hydroxyphenyl)acrylonitrile, or glycopyranosyl), C1-8 alkoxy, C1-4 alkyl, halogeno, ((C1-4 alkoxy)C1-4 alkoxy)C1-4 alkoxy, C2-8 acyloxy, C2-8 halogenoacyloxy, methylenedioxy, trifluoromethyl, phosphate group (-OP(O)(OH)2) or salt thereof, sulfate group (-OSO3H) or salt thereof, glycopyranosyl or salt thereof, a glycopyranosyl phosphate or salt thereof, glycopyranosyl sulfate or salt thereof, or piperidinopiperidinocarbonyloxy} or an ester or salt of the derivative THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD OS.CITING REF COUNT: 2 (3 CITINGS) REFERENCE COUNT: THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT => => s 15 not py>2003 7570071 PY>2003 L8 96 L5 NOT PY>2003 => focus PROCESSING COMPLETED FOR L8 96 FOCUS L8 1-=> d ibib abs hitstr ANSWER 1 OF 96 CAPLUS COPYRIGHT 2009 ACS on STN T.9 ACCESSION NUMBER: 1987:458571 CAPLUS DOCUMENT NUMBER: 107:58571 ORIGINAL REFERENCE NO.: 107:9717a,9720a TITLE: Application of organoelement compounds of the fifth and sixth groups in organic synthesis. Part 44. A facile synthesis of pentafluorophenyl olefins via an arsonium ylide AUTHOR(S): Shen, Yanchang; Qiu, Weiming CORPORATE SOURCE: Shanghai Inst. Org. Chem., Acad. Sin., Shanghai, Peop. Rep. China SOURCE: Synthesis (1987), (1), 65-6CODEN: SYNTBF; ISSN: 0039-7881 DOCUMENT TYPE: Journal LANGUAGE: English CASREACT 107:58571 OTHER SOURCE(S): Benzaldehydes were treated with C6F5CH:AsPh3(I) to give C6F5CH:CHR1 (R1 = Ph, halophenyl, O2NC6H4, anisyl, styryl, etc.). I was obtained from CH2:AsPh3 and C6F6. ΙT 19292-25-2P 37516-14-6P 37516-15-7P 78622-66-9P 109384-55-6P 109384-56-7P 109384-57-8P 109384-58-9P 109384-59-0P 109384-60-3P 109384-61-4P 109384-62-5P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) RN 19292-25-2 CAPLUS Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-phenylethenyl]- (CA INDEX NAME) CN

RN 37516-14-6 CAPLUS

CN Benzene, pentafluoro[(1E)-2-(4-nitrophenyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 37516-15-7 CAPLUS

CN Benzene, [(1E)-2-(4-chlorophenyl)ethenyl]pentafluoro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 78622-66-9 CAPLUS

CN Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-(4-methoxyphenyl)ethenyl]- (CA INDEX NAME)

RN 109384-55-6 CAPLUS

CN Benzene, [(1E)-2-(2-chlorophenyl)ethenyl]pentafluoro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 109384-56-7 CAPLUS

CN Benzene, pentafluoro[2-(4-fluorophenyl)ethenyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 109384-57-8 CAPLUS

CN Benzene, [2-(2,4-dichlorophenyl)] ethenyl]pentafluoro-, (E)- (9CI) (CA INDEX NAME)

RN 109384-58-9 CAPLUS

CN Benzene, 1-[(1E)-2-(4-bromophenyl)ethenyl]-2,3,4,5,6-pentafluoro- (CA INDEX NAME)

Double bond geometry as shown.

RN 109384-59-0 CAPLUS

CN Benzene, [2-(4-bromophenyl)ethenyl]pentafluoro-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 109384-60-3 CAPLUS

CN Benzene, pentafluoro[2-(4-methoxyphenyl)ethenyl]-, (Z)- (9CI) (CA INDEX NAME)

RN 109384-61-4 CAPLUS

CN 1,3-Benzodioxole, 5-[2-(pentafluorophenyl)ethenyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 109384-62-5 CAPLUS

CN 1,3-Benzodioxole, 5-[2-(pentafluorophenyl)ethenyl]-, (Z)- (9CI) (CA INDEX NAME)

=> fil reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	115.58	310.06
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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CA SUBSCRIBER PRICE	-13.94	-13.94

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STRUCTURE FILE UPDATES: 27 JUL 2009 HIGHEST RN 1169753-75-6 DICTIONARY FILE UPDATES: 27 JUL 2009 HIGHEST RN 1169753-75-6

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http://www.cas.org/support/stngen/stndoc/properties.html

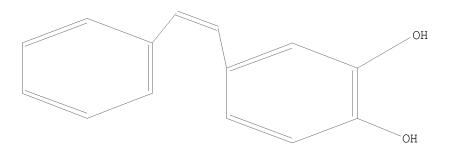
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13  14  15  16
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12
chain bonds :
5-13  9-14  11-16  12-15  13-14
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  8-9  9-10  10-11  11-12
exact/norm bonds :
11-16  12-15
exact bonds :
5-13  9-14  13-14
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  8-9  9-10  10-11  11-12
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Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS

=> d L10 HAS NO ANSWERS L10 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 110

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SAMPLE SCREEN SEARCH COMPLETED - 787 TO ITERATE

100.0% PROCESSED 787 ITERATIONS 22 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 14057 TO 17423 PROJECTED ANSWERS: 159 TO 721

L11 22 SEA SSS SAM L10

=> d scan

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneethanesulfonic acid, β -[(3,4-dihydroxyphenyl)methylene]-3,4-dimethoxy-

MF C17 H18 07 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):21

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 1,2,3-Benzenetriol, 5-[2-(3,5-dihydroxyphenyl)ethenyl]-, (Z)- (9CI) MF C14 H12 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

MF C23 H17 O2 S2 . C1 O4

CM 1

$$\begin{array}{c|c} Ph & & \\ & \\ S + & \\ & \\ OH & \\ \end{array}$$

CM 2

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, 4-(aminosulfonyl)- α -[(3,4-dihydroxyphenyl)methylene]-, 2-phenylethyl ester, (α E)-MF C23 H21 N O6 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Methanone, (4-benzoyl-1-piperazinyl)[4-[(1E)-2-(3,4-dihydroxyphenyl)ethenyl]phenyl]MF C26 H24 N2 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2(1H)-Pyrimidinone, 4-amino-1- β -D-arabinofuranosyl-, mixt. with 5,5'-(1,2-ethenediyl)bis[1,2,3-benzenetriol] (9CI)

MF C14 H12 O6 . C9 H13 N3 O5

CI MXS

CM 1

CM 2

Absolute stereochemistry.

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2(1H)-Pyrimidinone, 4-amino-1- β -D-arabinofuranosyl-, mixt. with 5-[2-(3,5-dihydroxyphenyl)ethenyl]-1,2,3-benzenetriol (9CI)

MF C14 H12 O5 . C9 H13 N3 O5

CI MXS

CM 1

CM 2

Absolute stereochemistry.

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzoic acid, 4-[2-[3,4-dihydroxy-5-(3-methyl-2-buten-1-yl)phenyl]ethenyl]-, methyl ester

MF C21 H22 O4

$$\begin{array}{c} \text{HO} \\ \text{HO} \\ \text{HO} \\ \text{Me}_2\text{C} = \text{CH} - \text{CH}_2 \\ \end{array} \begin{array}{c} \text{C} - \text{OMe} \\ \\ \text{O} \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Benzamide, 4-[2-(3,4-dihydroxyphenyl)ethenyl]-N,N-bis(2-hydroxyethyl)MF C19 H21 N O5

HO CH CH
$$=$$
 CH $=$ CH $=$ CH $=$ CH $_2$ CH $_2$ OH $=$ O CH $_2$ CH $_2$ OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid, 3,4-dichloro- α -[(3,4-dihydroxyphenyl)methylene]-MF C15 H10 C12 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetonitrile, 3,4-dihydroxy- α -[(4-hydroxy-3-iodo-5-methoxyphenyl)methylene]-, (α Z)-MF C16 H12 I N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenesulfonic acid, 2-[2-(4-ethenylphenyl)ethenyl]-4,5-dihydroxy-

MF C16 H14 O5 S

CI COM

$$CH$$
 CH CH CH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,2-Benzenediol, 4-[2-[3-(6-hydroxy-6-methylheptyl)phenyl]-

MF C22 H28 O3

HO CH CH (CH₂)
$$5$$
 C Me Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,2,3-Benzenetriol, 5,5',5'',5''',5'''',5''''-[1,3,5benzenetriyltris[(1E)-2,1-ethenediyl-4,1-phenylene-(1E)-2,1-ethenediyl5,1,3-benzenetriylbis[(1E)-2,1-ethenediyl-4,1-phenylene-(1E)-2,1ethenediyl]]]hexakis- (9CI)

MF C150 H114 O18

Double bond geometry as shown.

PAGE 1-A

НО

HO

PAGE 1-B

PAGE 1-C

PAGE 3-B

PAGE 3-C

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzenepropanoic acid, $\alpha-[[3-[2-[5-[1-carboxy-2-(3,4-dihydroxyphenyl)ethoxy]-2-(3,4-dihydroxyphenyl)-3-[2-[2-(3,4-dihydroxyphenyl)ethenyl]-3,4-dihydroxyphenyl]-5-oxo-1,3-pentadien-1-yl]-3,4-dihydroxyphenyl]-1-oxo-2-propen-1-yl]oxy]-3,4-dihydroxy-$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 1,2,4-Benzenetriol, 5-[2-(4-hydroxyphenyl)ethenyl]-MF C14 H12 O4

MF

C52 H42 O20

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetonitrile, 3,4-dihydroxy- α -(1-naphthalenylmethylene)-MF C19 H13 N O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetonitrile, 3,4-dihydroxy- α -(phenylmethylene)-MF C15 H11 N O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetonitrile, 4-chloro- α -[(3,4-dihydroxyphenyl)methylene]-MF C15 H10 Cl N O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,2-Benzenediol, 4-[(1E)-2-(3-hydroxy-5-methoxyphenyl)ethenyl]MF C15 H14 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2H-1-Benzopyran-3,7-diol, 4,4'-[2-[2-(3,4-dihydroxyphenyl)ethenyl]-4,6-dihydroxy-1,3-phenylene]bis[3,4-dihydro-2-(4-hydroxyphenyl)-, [2R-[2 α ,3 α ,4 β [E(2'R*,3'S*,4'S*)]]]- (9CI)

MF C44 H36 O12

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,2-Benzenediol, 4-[2-(3-hydroxyphenyl)ethenyl]-3-methoxy-

MF C15 H14 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s 110 full FULL SEARCH INITIATED 10:11:39 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 15465 TO ITERATE

100.0% PROCESSED 15465 ITERATIONS 412 ANSWERS

SEARCH TIME: 00.00.01

L12 412 SEA SSS FUL L10

=> fil capl

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FILE LAST UPDATED: 28 Jul 2009 (20090728/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

CAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2009.

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=> s 112

L13 1181 L12

=> a 113 and cancer

A IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> s 113 and cancer

414531 CANCER 60981 CANCERS 429588 CANCER

(CANCER OR CANCERS)

L14 111 L13 AND CANCER

=> s 114 not py>2002

8578358 PY>2002

L15 26 L14 NOT PY>2002

=> d ibib abs 25-26 hitstr

L15 ANSWER 25 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

1987:451278 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 107:51278

ORIGINAL REFERENCE NO.: 107:8347a,8350a

TITLE: Analysis of tamoxifen and its metabolites in human

plasma by gas chromatography-mass spectrometry (GC-MS)

using selected ion monitoring (SIM)

AUTHOR(S): Murphy, C.; Fotsis, T.; Pantzar, P.; Adlercreutz, H.;

Martin, F.

CORPORATE SOURCE: Dep. Pharmacol., Univ. Coll. Dublin, Dublin, Ire.

SOURCE: Journal of Steroid Biochemistry (1987), 26(5), 547-55

CODEN: JSTBBK; ISSN: 0022-4731

DOCUMENT TYPE: Journal LANGUAGE: English

A method for the anal. of tamoxifen and its metabolites in the plasma from AB tamoxifen-treated breast cancer patients, by capillary GC-MS

using selected ion monitoring, is described. Metabolite extraction was carried out on a Sep-pak C18 cartridge and metabolite purification by selective ion-exchange chromatog. steps. Satisfactory recovery of radioactive stds.

through the extraction and purification steps was obtained. The method was accurate

and precise with precision coefficient of variation values ranging from 4.3-11% for tamoxifen and its metabolites. Tamoxifen, 4-hydroxytamoxifen, metabolite Y and N-desmethyltamoxifen were identified with certainty in the plasma on the basis of GC relative retention times and mass spectral comparison with authentic stds.; because of their low abundance in the plasma cis-metabolite E and 3,4-dihydroxytamoxifen could only be tentatively identified but identical GC behavior and a satisfactory comparison of the abundance of key fragment ions was achieved. The tamoxifen and metabolite concentration ranges (ng/mL) in the group of patients who received 40 or 80 ng tamoxifen for 14 days were tamoxifen, 307-745;

N-desmethyltamoxifen, 185-491; 4-hydroxytamoxifen, 1.4-2.5; 3,4-dihydroxytamoxifen, 0.7-2.0; metabolite Y, 19.0-112; and metabolite E1, 0.9-2.0.

IT 81992-84-9, 3,4-Dihydroxytamoxifen

RL: ANT (Analyte); ANST (Analytical study)

(determination of, in blood plasma of humans, as tamoxifen metabolite, by

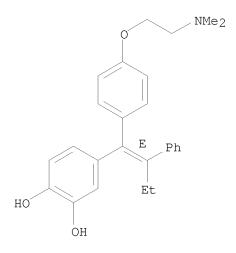
gas

chromatog.-mass spectrometry)

RN 81992-84-9 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (12 CITINGS)

L15 ANSWER 26 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1987:44185 CAPLUS

DOCUMENT NUMBER: 1967:44185

ORIGINAL REFERENCE NO.: 106:7209a,7212a

TITLE: Calmodulin antagonism and growth-inhibiting activity

of triphenylethylene antiestrogens in MCF-7 human

breast cancer cells

AUTHOR(S): Gulino, Alberto; Barrera, Giuseppina; Vacca,

Alessandra; Farina, Antonietta; Ferretti, Carlo;

Screpanti, Isabella; Dianzani, Mario U.; Frati, Luigi

CORPORATE SOURCE: Dip. Med. Sper., Univ. "La Sapienza", Rome, 00161,

Italy

SOURCE: Cancer Research (1986), 46(12, Pt. 1), 6274-8

CODEN: CNREA8; ISSN: 0008-5472

DOCUMENT TYPE: Journal LANGUAGE: English

The effects of the triphenylethylene antiestrogens tamoxifen [10540-29-1], N-demethyltamoxifen [31750-48-8], nafoxidine [1845-11-0], hydroxytamoxifen [68047-06-3], and 3,4-dihydroxytamoxifen [81992-84-9] on the inhibition of both calmodulin-dependent cAMP phosphodiesterase [9036-21-9] activity and proliferation of breast cancer cells (MCF-7) were studied. Hydroxylation of the triphenylethylene mol. decreased its ability to inhibit calmodulin-dependent phosphodiesterase activity in vitro. Furthermore, the growth-inhibiting activity of several antiestrogens and other calmodulin antagonists [R24571 [57265-65-3], trifluoperazine [117-89-5], N-(6-aminohexyl)-5-chloronaphthalene-1-sulfonamide [65595-90-6], and

N-(6-aminohexyl)-1-naphthalenesulfonamide [79458-81-4]] correlated with their antagonistic effects on calmodulin activity. The level of activity was: R24571 > tamoxifen = N-demethyltamoxiffen = nafoxidine > 4-hydroxytamoxifen > 3,4-dihydroxytamoxifen = trifluoperazine > N-(6-aminohexyl)-5-chloronaphthalene-1-sulfonamide > metabolite A > N-(6-aminohexyl)-1-naphthlenesulfonamide. However, the protein kinase C-activating and -inhibiting drugs (phorbol tetradecanoate 13-acetate and tamoxifen, resp.) had a synergistic inhibitory effect on MCF-7 cell growth. Thus, antiestrogen interactions with calmodulin, and not protein kinase C, may play a role in mediating the drug induced estrogen-independent inhibition of breast cancer cell growth.

IT 81992-84-9, 3,4-Dihydroxytamoxifen

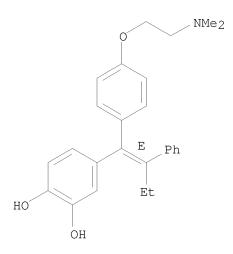
RL: BIOL (Biological study)

(mammary gland neoplasm growth inhibition by, of human, calmodulin antagonism mediation of)

RN 81992-84-9 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINGS)

=> d ibib abs hitstr 20-24

L15 ANSWER 20 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:169742 CAPLUS

DOCUMENT NUMBER: 130:346830

TITLE: The aromatase inactivator 4-hydroxyandrostenedione

(4-OH-A) inhibits tamoxifen metabolism by rat hepatic

cytochrome P-450 3A: potential for drug-drug interaction of tamoxifen and 4-OH-A in combined

anti-breast cancer therapy

AUTHOR(S): Dehal, Shangara S.; Brodie, Angela M. H.; Kupfer,

David

CORPORATE SOURCE: Department of Pharmacology and Molecular Toxicology,

University of Massachusetts Medical Center, Worcester,

MA, USA

SOURCE: Drug Metabolism and Disposition (1999), 27(3), 389-394

CODEN: DMDSAI; ISSN: 0090-9556

PUBLISHER: American Society for Pharmacology and Experimental

 ${\tt Therapeutics}$

DOCUMENT TYPE: Journal LANGUAGE: English

Tamoxifen (tam), an anti-breast cancer agent, is metabolized AB into tam-N-oxide by the hepatic flavin-containing monooxygenase and into N-desmethyl- and 4-hydroxy-tam by cytochrome P-450s (CYPs). Addnl., tam is metabolically activated by hepatic CYP3A, forming a reactive intermediate that binds covalently to proteins. Tam and 4-hydroxyandrostenedione (4-OH-A) are currently used to treat breast cancer, and it has been contemplated that 4-OH-A be given concurrently with tam to contravene potential tumor resistance to tam. Because alterations in tam metabolism may influence its therapeutic efficacy, the effect of 4-OH-A on tam metabolism was examined Incubation of tam with liver microsomes from phenobarbital-treated rats, in the presence of 4-OH-A (10-100 $\mu\text{M})\text{,}$ resulted in marked inhibition of tam-N-demethylation and tam covalent binding and in decreased tam-N-oxide accumulation; however, there was no inhibition of the formation of 4-hydroxy-tam and of 3,4-dihydroxytamoxifen. These findings indicate that 4-OH-A inhibits CYP3A, but not P 450(s) that catalyze tam 4-hydroxylation. The diminished tam-N-oxide accumulation could be due to decreased N-oxide formation and/or due to increased N-oxide reduction Incubation of tam-N-oxide with liver microsomes containing heat-inactivated flavin-containing monooxygenase

demonstrated that 4-OH-A increases the accumulation of tam, possibly by diminishing its P 450-mediated metabolism. Kinetic studies indicate that 4-OH-A is a competitive inhibitor of CYP3A, but not a time-dependent inactivator. Consequently, the concurrent treatment of tam and 4-OH-A may result in increased tam half-life and thus could potentiate the therapeutic efficacy of tam and diminish the potential side effects of tam by inhibiting its covalent binding to proteins and possibly to DNA.

IT 81992-84-9, 3,4-Dihydroxytamoxifen

RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)

(4-hydroxyandrostenedioneinhibits tamoxifen metabolism by rat hepatic cytochrome P 450 3A and potential for drug-drug interaction in combined anti-breast cancer therapy)

RN 81992-84-9 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS

L15 ANSWER 21 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:277674 CAPLUS

DOCUMENT NUMBER: 129:49604

ORIGINAL REFERENCE NO.: 129:10215a, 10218a

TITLE: Evaluation of the antioxidant potential of natural

products

AUTHOR(S): Lee, Sang Kook; Mbwambo, Zakaria H.; Chung, HaSook;

Luyengi, Lumonadio; Gamez, Esperanza J. C.; Mehta, Rajendra G.; Kinghorn, A. Douglas; Pezzuto, John M.

CORPORATE SOURCE: Program for Collaborative Research in the

Pharmaceutical Sciences, and Department of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, University of Illinois, Chicago, IL, 60612, USA

SOURCE: Combinatorial Chemistry and High Throughput Screening

(1998), 1(1), 35-46

CODEN: CCHSFU; ISSN: 1386-2073 Bentham Science Publishers

DOCUMENT TYPE: Journal LANGUAGE: English

PUBLISHER:

Since reactive oxygen radicals play an important role in carcinogenesis and other human disease states, antioxidants present in consumable fruits, vegetables, and beverages have received considerable attention as cancer chemopreventive agents. Thus, in order to identify antioxidants in plant exts., test materials were assessed for potential to scavenge stable 1,2-diphenyl-2-picrylhydrazyl (DPPH) free radicals, reduce TPA-induced free radical formation in cultured HL-60 human leukemia cells, and inhibit responses observed with a xanthine/xanthine oxidase assay system. Approx. 700 plant exts. were evaluated, and 28 were found to be active in the DPPJ free radical scavenging assay. Based on secondary analyses performed to assess inhibition of 7,12-dimethylbenz(a)anhracene-induced preneoplastic lesion formation with a mouse mammary organ culture model, Chorizanthe diffusa Benth. (Polygonaceae), Mezoneuron cucullatum Roxb. (Leguminosae), Cerbera manghas L. (Apocynaceae) and Daphniphyllum calycinum Benth. (Daphniphyllaceae) were selected and subjected to bioassay-quided fractionation. 5,7,3',5',-Tetrahydroxy-8,4'dimethoxyflavonol, 5,8,4'-trihydroxy-7,3'-dimethoxyflavonol, 5,3',4'-trihydroxy-7-methoxyflavonol, and 6,3',4'-trihydroxy-7-methoxyflavonol were identified as active principles from C. diffusa. Piceatannol, trans-resveratrol, apigenin and scirpusin A were found as the active principles of M. cucullatum, olivil, (-)-carinol, and (+)-cycloolivil were active principles from C. mangahas, and 5,6,7,4'-tetrahydroxyflavone 3-o-rutinoside and kaempferol 3-o-neohesperidoside were active principles from D. calycinum. Of these substances, the hydroxystilbenes piceatannol and trans-resveratrol have thus far been shown to inhibit carcinogen-induced preneoplastic lesion formation in the mouse mammary gland organ culture model.

IT 10083-24-6, Piceatannol

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(antioxidant potential of natural products)

RN 10083-24-6 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-2-(3,5-dihydroxyphenyl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

OS.CITING REF COUNT: 108 THERE ARE 108 CAPLUS RECORDS THAT CITE THIS

RECORD (108 CITINGS)

REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 22 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:155442 CAPLUS

DOCUMENT NUMBER: 124:251181

ORIGINAL REFERENCE NO.: 124:46277a, 46280a

TITLE: Evidence that the catechol 3,4-dihydroxytamoxifen is a

proximate intermediate to the reactive species binding

covalently to proteins

AUTHOR(S): Dehal, Shangara S.; Kupfer, David

CORPORATE SOURCE: Worcester Foundation for Biomedical Research,

Shrewbury, MA, 01545, USA

SOURCE: Cancer Research (1996), 56(6), 1283-90

CODEN: CNREA8; ISSN: 0008-5472

PUBLISHER: American Association for Cancer Research

DOCUMENT TYPE: Journal LANGUAGE: English

AB Metabolism of tamoxifen by rat and human hepatic microsomal cytochrome P450s (CYPs) forms a reactive intermediate that irreversibly binds to microsomal proteins (C. Mani and D. Kupfer, Cancer Res., 51: 6052-6058, 1991). The current study examines intermediate(s). The rate of covalent binding of tamoxifen metabolites, tamoxifen N-oxide, N-desmethyltamoxifen, and tamoxifen N-oxide-epoxide was approx. equal to or less than that of tamoxifen. By contrast, covalent binding of 4-hydroxytamoxifen (3-OH-tam) was 3-5-fold higher than that of tamoxifen, indicating that among the metabolites examined, 4-OH-tam or its metabolite(s) is most proximate to the reactive intermediate(s). Incubations of 4-OH-tam with liver microsomes from PCN-treated rats yielded three detectable metabolites. One was identified as 4-OH-tam N-oxide via its facile reduction back to 4-OH-tam by titanium(III) chloride. Another metabolite of 4-OH-tam, assumed to be 3,4-dihydroxytamoxifen (3,4-di-OH-tam) catechol, was demonstrated by its monomethylation with [3H]S-adenosyl-L-methionine ([3H]SAM) in the presence of endogenous catechol-O-methyltransferase. Monomethylated catechol from 4-OH-tam was formed at a 3-4-fold higher rate than from tamoxifen. It was reasoned that if the catechol is the most proximate metabolite to the reactive intermediate, then its methylation would reduce the formation of the reactive intermediate and result in a lower rate of covalent binding. In fact, addition of radio-inert SAM to incubations of tamoxifen inhibited covalent binding by 17-23%. By contrast, inclusion of 1.0 mM S-adenosyl-L-homocysteine, a potent inhibitor of catechol-O-methyltransferase-mediated methylation of 3,4-di-OH-tam, essentially overcame the inhibition of the covalent binding by SAM. Addnl., ascorbic acid and glutathione, inhibitors of covalent binding of tamoxifen, produced an elevation of methylated catechol. These findings

collectively indicate that 3,4-di-OH-tam is proximate to the ultimate reactive intermediate that results in covalent binding to microsomal proteins.

81992-84-9, 3,4-Dihydroxytamoxifen ΙT

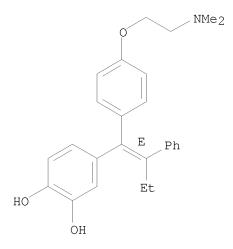
> RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)

(3,4-dihydroxytamoxifen is the tamoxifen metabolite proximate to the reactive intermediate that results in protein binding)

RN 81992-84-9 CAPLUS

1,2-Benzenediol, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-CN buten-1-y1]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 43 THERE ARE 43 CAPLUS RECORDS THAT CITE THIS RECORD (43 CITINGS)

L15 ANSWER 23 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:289266 CAPLUS

DOCUMENT NUMBER: 120:289266

ORIGINAL REFERENCE NO.: 120:50679a,50682a

TITLE: Analysis of phase I and phase II metabolites of

tamoxifen in breast cancer patients

AUTHOR(S): Poon, G. K.; Chui, Y. C.; McCague, R.; Loenning, P.

E.; Feng, R.; Rowlands, M. G.; Jarman, M.

CORPORATE SOURCE: Drug Dev. Sect., Inst. Cancer Res.,

Belmont/Sutton/Surrey, SM2 5NG, UK

Drug Metabolism and Disposition (1993), 21(6), 1119-24 SOURCE:

CODEN: DMDSAI; ISSN: 0090-9556

DOCUMENT TYPE: Journal LANGUAGE: English

AΒ This study describes the application of LC/MS/MS to the determination of phase Ι

and phase II metabolites of tamoxifen in urine and plasma samples of breast cancer patients. In the plasma exts., in addition to the parent drug and N-desmethyltamoxifen, a minor metabolite tamoxifen N-oxide was identified for the first time in human. Four intact glucuronides of tamoxifen metabolites were isolated in the 24-h posttreatment urine sample. They were the glucuronides of 4-hydroxytamoxifen, 4-hydroxy-N-desmethyltamoxifen, dihydroxytamoxifen, and a monohydroxy-N-desmethyltamoxifen. Hydroxylation followed by glucuronidation is a well-estimated metabolic route of tamoxifen, and this study describes for the first time direct analyses of these metabolites in human urine samples using online LC tandem MS.

IT 155144-62-0

RL: ANT (Analyte); ANST (Analytical study) (determination of, as metabolite, in blood plasma and urine of humans with breast cancer, by HPLC-mass spectrometry)

RN 155144-62-0 CAPLUS

CN β -D-Glucopyranosiduronic acid, 4(or 5)-[1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2-

hydroxyphenyl, (E)- (9CI) (CA INDEX NAME)

CM 1

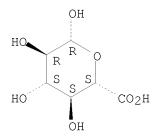
CRN 81992-84-9 CMF C26 H29 N O3

Double bond geometry as shown.

CM 2

CRN 23018-83-9 CMF C6 H10 O7

Absolute stereochemistry.



OS.CITING REF COUNT: 49 THERE ARE 49 CAPLUS RECORDS THAT CITE THIS RECORD (49 CITINGS)

L15 ANSWER 24 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1991:655797 CAPLUS

DOCUMENT NUMBER: 115:255797

ORIGINAL REFERENCE NO.: 115:43481a,43484a

TITLE: Preparation and use of catechol derivatives as medical

antioxidants

INVENTOR(S): Korkolainen, Tapio Juhani; Nissinen, Erkki Aarne

Olavi; Backstrom, Reijo Johannes; Pippuri, Aino

Kyllikki

PATENT ASSIGNEE(S): Orion-Yhtyma Oy, Finland SOURCE: Eur. Pat. Appl., 14 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 444899 EP 444899	A2 A3	19910904 19921125	EP 1991-301587	19910227
EP 444899	B1	19970205		Ω Π
			B, GR, IT, LI, LU, NL	
JP 04211627 JP 3157846	A B2	19920803 20010416	JP 1991-30908	19910226
AT 148626	T	19970215	AT 1991-301587	19910227
HR 9201250	В1	20000630	HR 1992-1250	19921112
US 5489614	A	19960206	US 1995-461752	19950605
PRIORITY APPLN. INFO.:			YU 1989-21	A 19890106
			GB 1990-4348	A 19900227
			FI 1986-4875	A 19861128
			GB 1987-12437	A 19870528
			US 1987-126911	A3 19871127
			US 1988-288979	A2 19881223
			US 1990-587791	A2 19900925
			US 1991-658666	B1 19910221
			US 1994-294762	B1 19940823
OTHER COHROL (C).	MADDAT	116.066707		

OTHER SOURCE(S): MARPAT 115:255797

Ι

GΙ

The title compds. [I; R2 = CH:CR3R4, CH2CHR3R4; R3 = acyl, cyclopropylcarbonyl; R4 = (un)substituted aryl, cyclopropylcarbonyl; X = halo, NO2, cyano, CF3, CHO, CO2H], their physiol. acceptable salts and esters, are claimed. Also claimed are the use of the known I (R2 = H, substituted alkyl, alkoxy, aryl, heterocyclyl, NO2, cyano, CHO, CO2H, CH:CR3R4, CH2CHR3R4; broader definitions for R3, R4 are given; X as above] and of their physiol. acceptable salts and esters for the prophylaxis and treatment of tissue damage induced in lipid peroxidn., e.g., in heart disease, rheumatoid arthritis, cancer, etc. Thus, a solution of Me2CHCOCH2Ph and 3,4,5-(HO)2(O2N)C6H2CHO in Me2CHOH was saturated by HCl(g) at 20° and stirred 4 h at room temperature to give title compound I (R2 = Me2CHCOCPh:CH, X = O2N). The latter in a controlled peroxidn. test in vitro had a stoichiometric factor 3.3 vs 2.0 for Trolox and 0.7 for ascorbic acid.

 (preparation of, as medical antioxidant)

RN 137419-33-1 CAPLUS

CN 1-Penten-3-one, 1-(3,4-dihydroxy-5-nitrophenyl)-4-methyl-2-phenyl- (CA INDEX NAME)

RN 137419-37-5 CAPLUS

CN 3-Buten-2-one, 4-(3,4-dihydroxy-5-nitrophenyl)-3-phenyl- (CA INDEX NAME)

RN 137419-38-6 CAPLUS

CN 3-Buten-2-one, 4-(3,4-dihydroxy-5-nitrophenyl)-3-(4-methylphenyl)- (CA INDEX NAME)

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

=> d ibib abs hitstr 15-19

L15 ANSWER 15 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:808259 CAPLUS

DOCUMENT NUMBER: 134:97896

TITLE: Mappain, a new cytotoxic prenylated stilbene from

Macaranga mappa

AUTHOR(S): van der Kaaden, Jacobus E.; Hemscheidt, Thomas K.;

Mooberry, Susan L.

CORPORATE SOURCE: Department of Chemistry, University of Hawaii at

Manoa, Honolulu, HI, 96822, USA

SOURCE: Journal of Natural Products (2001), 64(1), 103-105

CODEN: JNPRDF; ISSN: 0163-3864

American Chemical Society

Journal English

GΙ

PUBLISHER:

LANGUAGE:

DOCUMENT TYPE:

AB A new prenylated stilbene, mappain (I), was isolated from leaves of Macaranga mappa by bioassay-guided fractionation. The structure was established by application of spectroscopic methods. Mappain is cytotoxic but it appears to be a poor substrate for P-glycoprotein-mediated transport because it is equally potent and effective against the drug-sensitive SK-OV-3 and drug-resistant SKVLB-1 ovarian cancer cell lines, exhibiting an IC50 value of 1.3 μ M in both cases. IT 319915-14-5P, Mappain

Ι

319915-14-5P, Mappain
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(cytotoxic prenylated stilbene from Macaranga mappa)

RN 319915-14-5 CAPLUS

CN 1,2-Benzenediol, 5-[(1E)-2-[3,5-dihydroxy-4-(3-methyl-2-buten-1-yl)phenyl]ethenyl]-3-[(2E)-3,7-dimethyl-2,6-octadien-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

OS.CITING REF COUNT: THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD

(7 CITINGS)

12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT:

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 16 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:801085 CAPLUS

DOCUMENT NUMBER: 132:175303

TITLE: Synthesis and Reactivity of a Potential Carcinogenic

Metabolite of Tamoxifen:

3,4-Dihydroxytamoxifen-o-quinone

Zhang, Fagen; Fan, Peter W.; Liu, Xuemei; Shen, Lixin; AUTHOR(S):

Van Breemen, Richard B.; Bolton, Judy L.

CORPORATE SOURCE: Department of Medicinal Chemistry and Pharmacognosy

(M/C 781) College of Pharmacy, University of Illinois

at Chicago, Chicago, IL, 60612-7231, USA

Chemical Research in Toxicology (2000), 13(1), 53-62 SOURCE:

CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

Although tamoxifen is approved for the treatment of hormone-dependent breast cancer as well as for the prevention of breast cancer in high-risk women, several studies in animal models have shown that tamoxifen is hepatocarcinogenic, and in humans, tamoxifen has been associated with an increased risk of endometrial cancer. One potential mechanism of tamoxifen carcinogenesis could involve metabolism of tamoxifen to 3,4-dihydroxytamoxifen followed by oxidation to a highly reactive o-quinone which has the potential to alkylate and/or oxidize cellular macromols. in vivo. In the study presented here, the authors synthesized the 3,4-dihydroxytamoxifen, prepared its o-quinone chemical and enzymically, and studied the reactivity of the o-quinone with GSH and deoxynucleosides. The E (trans) and Z (cis) isomers of 3,4-dihydroxytamoxifen were synthesized using a concise synthetic pathway (four steps). This approach is based on the McMurry reaction between the key 4-(2-chloroethoxy)-3,4-methylenedioxybenzophenone and propiophenone, followed by selective removal of the methylenedioxy ring of (E,Z)-1-[4-[2-(N,N-dimethylamino)ethoxy]phenyl]-1-(3,4methylenedioxyphenyl)-2-phenyl-1-butene with BCl3. Oxidation of 3,4-dihydroxytamoxifen by activated silver oxide or tyrosinase gave 3,4-dihydroxytamoxifen-o-quinone as a mixture of E and Z isomers. The resulting o-quinone has a half-life of approx. 80 min under physiol. conditions. Reaction of the o-quinone with GSH gave two di-GSH conjugates and three mono GSH conjugates. Incubation of 3,4-dihydroxytamoxifen with GSH in the presence of microsomal P 450 gave the same GSH conjugates which were also detected in incubations with human breast cancer cells (MCF-7). Reaction of 3,4-dihydroxytamoxifen-o-quinone with deoxynucleosides gave only thymidine and deoxyguanosine adducts; neither deoxyadenosine nor deoxycytosine adducts were detected. Preliminary studies conducted with human breast cancer cell lines showed that 3,4-dihydroxytamoxifen exhibited cytotoxic potency similar to that of 4-hydroxytamoxifen and tamoxifen in an estrogen receptor neg. (ER-) cell line (MDA-MB-231); however, in the ER+ cell line (MCF-7), the catechol metabolite was about half as toxic as the other two compds. Finally, in the presence of microsomes and GSH, 4-hydroxytamoxifen gave predominantly quinone methide GSH conjugates as reported in the previous paper in this issue [Fan, P. W., et al. (2000) Chemical Res. Toxicol. 13, XX-XX]. However, in the presence of tyrosinase and GSH, 4-hydroxytamoxifen was primarily converted to o-quinone GSH conjugates. These results suggest that the catechol metabolite of tamoxifen has the potential to cause cytotoxicity in vivo through formation of 3,4-dihydroxytamoxifen-o-quinone. ΤТ

(E)-3, 4-Dihydroxytamoxifen

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(synthesis and reactivity of a potential carcinogenic metabolite of tamoxifen dihydroxytamoxifen-o-quinone in relation to breast cancer inhibition)

RN 65319-40-6 CAPLUS

CN 1,2-Benzenediol, 4-[(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

RN 81992-84-9 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

IT 259149-80-9 259149-81-0 259149-82-1
RL: BSU (Biological study, unclassified); FMU (Formation, unclassified);
MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)

(synthesis and reactivity of a potential carcinogenic metabolite of

tamoxifen dihydroxytamoxifen-o-quinone in relation to breast cancer inhibition)

RN 259149-80-9 CAPLUS

CN Glycine, $L-\gamma$ -glutamyl-S-[5-[(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 259149-81-0 CAPLUS

CN Glycine, $L-\gamma$ -glutamyl-S-[5-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

RN 259149-82-1 CAPLUS

CN Glycine, 2,2',2''-[3-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-5,6-dihydroxy-1,2,4-benzenetriyl]tris[L- γ -glutamyl-L-cysteinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

IT 259149-75-2

RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative) (synthesis and reactivity of a potential carcinogenic metabolite of

tamoxifen dihydroxytamoxifen-o-quinone in relation to breast cancer inhibition)

RN 259149-75-2 CAPLUS

CN Glycine, 2,2',2''-[3-[(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-5,6-dihydroxy-1,2,4-benzenetriyl]tris[L- γ -glutamyl-L-cysteinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

IT 259149-73-0 259149-74-1 259149-76-3 259149-77-4 259149-78-5 259149-79-6

RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative) (synthesis and reactivity of a potential carcinogenic metabolite of tamoxifen dihydroxytamoxifen-o-quinone in relation to breast cancer inhibition)

RN 259149-73-0 CAPLUS

CN L-Cysteine, S-[5-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]-2,3-dihydroxyphenyl]- (CA INDEX NAME)

RN 259149-74-1 CAPLUS

CN L-Cysteine, S-[5-[(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]-2,3-dihydroxyphenyl]- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 259149-76-3 CAPLUS

CN Thymidine, 3'-deoxy-3-[5-[(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl]-1-butenyl]-2, <math>3-dihydroxyphenyl]-(9CI) (CA INDEX NAME)

RN 259149-77-4 CAPLUS

CN Thymidine, 3'-deoxy-3-[5-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl]-1-butenyl]-2, <math>3-dihydroxyphenyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 259149-78-5 CAPLUS

CN Guanosine, 3'-deoxy-N-[5-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]- (9CI) (CA INDEX NAME)

RN 259149-79-6 CAPLUS

CN Guanosine, 3'-deoxy-N-[5-[(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

OS.CITING REF COUNT: 39 THERE ARE 39 CAPLUS RECORDS THAT CITE THIS

RECORD (39 CITINGS)

REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 17 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:796363 CAPLUS

DOCUMENT NUMBER: 132:160795

TITLE: 4-Hydroxylated Metabolites of the Antiestrogens

Tamoxifen and Toremifene Are Metabolized to Unusually

Stable Quinone Methides

AUTHOR(S): Fan, Peter W.; Zhang, Fagen; Bolton, Judy L.

CORPORATE SOURCE: Department of Medicinal Chemistry and Pharmacognosy

(M/C 781) College of Pharmacy, University of Illinois

at Chicago, Chicago, IL, 60612-7231, USA

SOURCE: Chemical Research in Toxicology (2000), 13(1), 45-52

CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

Tamoxifen is widely prescribed for the treatment of hormone-dependent breast cancer, and it has recently been approved by the Food and Drug Administration for the chemoprevention of this disease. However, long-term usage of tamoxifen has been linked to increased risk of developing endometrial cancer in women. One of the suggested pathways leading to the potential toxicity of tamoxifen involves its oxidative metabolism to 4-hydroxytamoxifen, which may be further oxidized to an electrophilic quinone methide. The resulting quinone methide has the potential to alkylate DNA and may initiate the carcinogenic process. To further probe the chemical reactivity and toxicity of such an electrophilic species, the authors have prepared the 4-hydroxytamoxifen quinone methide chemical and enzymically, examined its reactivity under physiol. conditions, and quantified its reactivity with GSH. Interestingly, this quinone methide is unusually stable; its half-life under physiol. conditions is approx. 3 h, and its half-life in the presence of GSH is approx. 4 min. The reaction between 4-hydroxytamoxifen quinone methide and GSH appears to be a reversible process because the quinone methide GSH conjugates slowly decompose over time, regenerating the quinone methide as indicated by LC/MS/MS data. The tamoxifen GSH conjugates were detected in microsomal incubations with 4-hydroxytamoxifen; however, none were observed in breast cancer cell lines (MCF-7) perhaps because very little quinone methides is formed. Toremifene, which is a chlorinated analog of tamoxifen, undergoes similar oxidative metabolism to give 4-hydroxytoremifene, which is further oxidized to the corresponding quinone methide. The toremifene quinone methide has a half-life of approx. 1 h under physiol. conditions, and its rate of reaction in the presence of excess GSH is approx. 6 min. More detailed analyses have indicated that the 4-hydroxytoremifene quinone methide reacts with two mols. of GSH and loses chlorine to give the corresponding di-GSH conjugates. The reaction mechanism likely involves an episulfonium ion intermediate which may contribute to the potential cytotoxic effects of toremifene. Similar to what was observed with 4-hydroxytamoxifen, 4-hydroxytoremifene was metabolized to di-GSH conjugates in microsomal incubations at about 3 times the rate of 4-hydroxytamoxifen, although no conjugates were detected with MCF-7 cells. Finally, these data suggest that quinone methide formation may not make a significant contribution to the cytotoxic and genotoxic effects of tamoxifen and toremifene.

IT 81992-84-9, 3,4-Dihydroxytamoxifen

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(hydroxylated metabolites of antiestrogens tamoxifen and toremifene are metabolized to unusually stable quinone methides in relation to conjugate formation with GSH and carcinogenicity)

RN 81992-84-9 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

IT 259087-29-1

RL: BSU (Biological study, unclassified); FMU (Formation, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)

(hydroxylated metabolites of antiestrogens tamoxifen and toremifene are metabolized to unusually stable quinone methides in relation to conjugate formation with GSH and carcinogenicity)

RN 259087-29-1 CAPLUS

CN Glycine, $L-\gamma$ -glutamyl-S-[3-(3,4-dihydroxyphenyl)-3-[4-[2-(dimethylamino)ethoxy]phenyl]-1-methyl-2-phenyl-2-propenyl]-L-cysteinyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

OS.CITING REF COUNT: 50 THERE ARE 50 CAPLUS RECORDS THAT CITE THIS

RECORD (52 CITINGS)

REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 18 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:467829 CAPLUS

DOCUMENT NUMBER: 131:266661

TITLE: Piceatannol, a stilbene phytochemical, inhibits

mitochondrial F0F1-ATPase activity by targeting the F1

complex

AUTHOR(S): Zheng, Jianbiao; Ramirez, Victor D.

CORPORATE SOURCE: Department of Molecular and Integrative Physiology,

University of Illinois at Urbana-Champaign, Urbana,

IL, 61801, USA

SOURCE: Biochemical and Biophysical Research Communications

(1999), 261(2), 499-503

CODEN: BBRCA9; ISSN: 0006-291X

PUBLISHER: Academic Press

DOCUMENT TYPE: Journal LANGUAGE: English

Piceatannol is a stilbene phytochem. from the seeds of Euphorbia lagascae, previously identified as an antileukemic principle. Piceatannol is considered an inhibitor of several tyrosine kinases. We recently reported that resveratrol, another stilbene phytoalexin from grape seeds, was an inhibitor of ATP synthase. Here, we demonstrated that piceatannol potently inhibited the rat brain mitochondrial F0F1-ATPase activity in both solubilized and submitochondrial prepns. (IC50 of 8-9 μM), while having relatively small effect on the Na+, K+-ATPase activity of porcine cerebral cortex (no effect up to 7 μM). Piceatannol inhibited the ATPase activity of the purified rat liver F1 with IC50 of about 4 μ M, while resveratrol was slightly less active (IC50 of about 14 μM). Our results indicate that piceatannol and resveratrol inhibit the F-type ATPase by targeting the F1 sector, which is located to the inner membrane of mitochondria and plasma membrane of normal endothelial cells and several cancer cell lines. This mechanism could potentially contribute to the multiple effects of these chemopreventive phytochems. (c) 1999 Academic Press.

IT 10083-24-6, Piceatannol

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(piceatannol inhibits mitochondrial F0F1-ATP as activity by targeting the F1 complex)

RN 10083-24-6 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-2-(3,5-dihydroxyphenyl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

OS.CITING REF COUNT: 55 THERE ARE 55 CAPLUS RECORDS THAT CITE THIS

RECORD (55 CITINGS)

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 19 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:379085 CAPLUS

DOCUMENT NUMBER: 131:169463

TITLE: Determination of Stilbenes (trans-Astringin, cis- and

trans-Piceid, and cis- and trans-Resveratrol) in

Portuguese Wines

AUTHOR(S): Ribeiro de Lima, Maria T.; Waffo-Teguo, Pierre;

Teissedre, Pierre L.; Pujolas, Agnes; Vercauteren,

Joseph; Cabanis, Jean C.; Merillon, Jean M.

CORPORATE SOURCE: Faculte des Sciences Pharmaceutiques Centre de

Formation et de Recherche en Enologie, Universite de

Montpellier I, Montpellier, 34060, Fr.

SOURCE: Journal of Agricultural and Food Chemistry (1999),

47(7), 2666-2670

CODEN: JAFCAU; ISSN: 0021-8561

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

AB Stilbenes have been shown to have cancer chemopreventive

activity and to protect lipoproteins from oxidative damage. A method is described for their direct determination in different types of wine using HPLC with UV detection. In a survey of 120 com. wines from Portugal and France, the highest concns. of stilbenes were found in red wines. The glucosides of resveratrol were present in higher concns. than the free isomers. Isolation from wine and characterization of trans-astringin in a

large quantity are described for the 1st time.

IT 29884-49-9

RL: ANT (Analyte); ANST (Analytical study)

(determination of stilbenes in Portuguese wines)

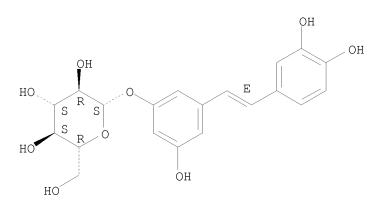
RN 29884-49-9 CAPLUS

CN β -D-Glucopyranoside, 3-[(1E)-2-(3,4-dihydroxyphenyl)ethenyl]-5-

hydroxyphenyl (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



OS.CITING REF COUNT: 32 THERE ARE 32 CAPLUS RECORDS THAT CITE THIS

RECORD (32 CITINGS)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L15 ANSWER 10 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:57665 CAPLUS

DOCUMENT NUMBER: 137:163396

TITLE: Ellagic acid inhibits nucleoside diphosphate kinase-B

activity

AUTHOR(S): Malmquist, N. A.; Anzinger, J. J.; Hirzel, D.; Buxton,

I. L. O.

CORPORATE SOURCE: Department of Pharmacology, University of Nevada

School of Medicine, Reno, NV, 89557, USA

Proceedings of the Western Pharmacology Society

(2001), $4\overline{4}$, 57-59

CODEN: PWPSA8; ISSN: 0083-8969 Western Pharmacology Society

DOCUMENT TYPE: Journal LANGUAGE: English

SOURCE:

PUBLISHER:

AB Various compds. that have anti-antiangiogenesis or general anti-cancer properties, such as polyphenolic tea compds., nucleoside analogs AZT, PAPS, and 8-Cl-cAMP, and ellagic acid, were examined for their ability to inhibit nucleoside diphosphate kinase-B (NDPK-B) activity.

NDPK-B activity was inhibited by the polyphenolic constituents of tea, i.e., EGCG, ECG and theaflavins. The nucleoside analogs, 8-Cl-cAMP and

NDPK-B activity was inhibited by the polyphenolic constituents of tea, i.e., EGCG, ECG and theaflavins. The nucleoside analogs, 8-Cl-cAMP and PAPS, inhibited NDPK-B transphosphorylation activity at relatively low potency. Ellagic acid (hexahydroxydiphenic acid dilactone), found through a structure search based on the conserved moiety contained in the most potent NDPK-B inhibiting polyphenolic tea compds., had the highest affinity of NDPK-B.

IT 10083-24-6, Piceatannol

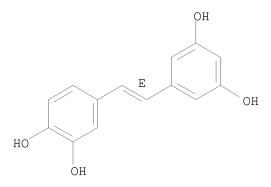
RL: PAC (Pharmacological activity); BIOL (Biological study)

(effects of tea polyphenols and nucleoside analogs on nucleoside diphosphate kinase-B activity)

RN 10083-24-6 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-2-(3,5-dihydroxyphenyl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD

(5 CITINGS)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 11 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:855006 CAPLUS

DOCUMENT NUMBER: 136:128734

TITLE: Synthesis and Reactivity of Potential Toxic

Metabolites of Tamoxifen Analogues: Droloxifene and

Toremifene o-Quinones

AUTHOR(S): Yao, Dan; Zhang, Fagen; Yu, Linning; Yang, Yanan; van

Breemen, Richard B.; Bolton, Judy L.

CORPORATE SOURCE: Department of Medicinal Chemistry and Pharmacognosy

(M/C 781) College of Pharmacy, University of Illinois

at Chicago, Chicago, IL, 60612-7231, USA

SOURCE: Chemical Research in Toxicology (2001), 14(12),

1643-1653

CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

Tamoxifen remains the endocrine therapy of choice in the treatment of all AB stages of hormone-dependent breast cancer. However, tamoxifen has been shown to increase the risk of endometrial cancer which has stimulated research for new effective antiestrogens, such as droloxifene and toremifene. In this study, the potential for these compds. to cause cytotoxic effects was investigated. One potential cytotoxic mechanism could involve metabolism of droloxifene and toremifene to catechols, followed by oxidation to reactive o-quinones. Another cytotoxic pathway could involve the oxidation of 4-hydroxytoremifene to an electrophilic quinone methide. Comparison of the amts. of GSH conjugates formed from 4-hydroxytamoxifen, droloxifene, and 4-hydroxytoremifene suggested that 4-hydroxytoremifene is more effective at formation of a quinone methide. However, all three substrates formed similar amts. of o-quinones. Both the tamoxifen-o-quinone and toremifene-o-quinone reacted with deoxynucleosides to give corresponding adducts. However, the toremifene-o-quinone was shown to be considerably more reactive than the tamoxifen-o-quinone in terms of both kinetic data as well as the yield and type of deoxynucleoside adducts formed. Since thymidine formed the most abundant adducts with the toremifene-o-quinone, sufficient material was obtained for characterization by 1H NMR, COSY-NMR, DEPT-NMR, and tandem mass spectrometry. Cytotoxicity studies with tamoxifen, droloxifene, 4-hydroxytamoxifen, 4-hydroxytoremifene, and their catechol metabolites were carried out in the human breast cancer cell lines S30 and MDA-MB-231. All of the metabolites tested showed cytotoxic effects that were similar to the parent antiestrogens which suggests that o-quinone formation from tamoxifen, droloxifene, and 4-hydroxytoremifene is unlikely to contribute to their cytotoxicity. However, the fact that the o-quinones formed adducts with deoxynucleosides in vitro implies that the o-quinone pathway might contribute to the genotoxicity of the antiestrogens in vivo.

IT 259149-80-9 259149-81-0 392710-66-6 392725-33-6 392725-34-7 392725-35-8

RL: BSU (Biological study, unclassified); BIOL (Biological study) (synthesis and reactivity of toxic metabolites of tamoxifen analogs, droloxifene and toremifene o-quinones)

RN 259149-80-9 CAPLUS

CN

Glycine, $L-\gamma$ -glutamyl-S-[5-[(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

RN 259149-81-0 CAPLUS

CN Glycine, $L-\gamma$ -glutamyl-S-[5-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 392710-66-6 CAPLUS

CN Thymidine, 3-[5-[(1E)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl]-1-butenyl]-2, 3-dihydroxyphenyl]- (9CI) (CA INDEX NAME)

RN 392725-33-6 CAPLUS

CN Glycine, 2,2'-[[(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]dihydroxyphenylene]bis[L- γ -glutamyl-L-cysteinyl- (9CI) (CA INDEX NAME)

RN 392725-34-7 CAPLUS

CN Glycine, 2,2'-[[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]dihydroxyphenylene]bis[L- γ -glutamyl-L-cysteinyl- (9CI) (CA INDEX NAME)

RN 392725-35-8 CAPLUS

CN Glycine, $L-\gamma$ -glutamyl-S-[[1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]dihydroxyphenyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

IT 392710-51-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(synthesis and reactivity of toxic metabolites of tamoxifen analogs, droloxifene and toremifene o-quinones)

RN 392710-51-9 CAPLUS

CN 1,2-Benzenediol, 4-[(1Z)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

IT 81992-84-9, 3,4-Dihydroxytamoxifen

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(synthesis and reactivity of toxic metabolites of tamoxifen analogs, droloxifene and toremifene o-quinones)

RN 81992-84-9 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

IT 392710-49-5P 392710-55-3P 392710-57-5P 392710-58-6P 392710-60-0P 392710-61-1P 392725-30-3P 392725-31-4P 392725-32-5P 392725-36-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis and reactivity of toxic metabolites of tamoxifen analogs, droloxifene and toremifene o-quinones)

RN 392710-49-5 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

RN 392710-55-3 CAPLUS CN Glycine, $L-\gamma$ -glutamyl-S-[5-[(1Z)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

RN 392710-57-5 CAPLUS

CN Glycine, $L-\gamma$ -glutamyl-S-[5-[(1E)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 392710-58-6 CAPLUS

CN Glycine, 2,2',2''-[3-[(1Z)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-5,6-dihydroxy-1,2,4-benzenetriyl]tris[L- γ -glutamyl-L-cysteinyl- (9CI) (CA INDEX NAME)

RN 392710-60-0 CAPLUS CN Glycine, 2,2',2''-[3-[(1E)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-5,6-dihydroxy-1,2,4-benzenetriyl]tris[L- γ -glutamyl-L-cysteinyl- (9CI) (CA INDEX NAME)

RN 392710-61-1 CAPLUS

CN Thymidine, 3-[5-[(1Z)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 392725-30-3 CAPLUS

CN Glycine, $L-\gamma$ -glutamyl-S-[[4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]dihydroxyphenyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} \\ & \text{C1CH}_2-\text{CH}_2-\text{C} \\ \text{Me}_2\text{N}-\text{CH}_2-\text{CH}_2-\text{O} \\ & \text{C} \end{array} \quad \begin{array}{c|c} \text{OH} \\ & \text{OH} \\ \end{array}$$

RN 392725-31-4 CAPLUS

CN Glycine, 2,2'-[[(1Z)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]dihydroxyphenylene]bis[L- γ -glutamyl-L-cysteinyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} \\ & \text{C1CH}_2\text{--CH}_2\text{--C} & \text{OH} \\ \text{Me}_2\text{N}\text{--CH}_2\text{--CH}_2\text{--O} & \text{OH} \\ \end{array}$$

RN 392725-32-5 CAPLUS

CN Guanosine, N-[[(1Z)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]dihydroxyphenyl]-2'-deoxy- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} \\ & \text{C1CH}_2\text{--}\text{CH}_2\text{--}\text{C} \\ & \text{OH} \\ \\ \text{Me}_2\text{N}\text{--}\text{CH}_2\text{--}\text{CH}_2\text{--}\text{O} \\ & \text{C} \end{array}$$

D1-NH
$$\stackrel{N}{H}$$
 $\stackrel{N}{N}$ OH

RN 392725-36-9 CAPLUS

CN Glycine, 2,2'-[[(1E)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]dihydroxyphenylene]bis[L- γ -glutamyl-L-cysteinyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} \\ & \text{ClCH}_2\text{--CH}_2\text{--C} & \text{OH} \\ \text{Me}_2\text{N}\text{--CH}_2\text{--CH}_2\text{--O} & \text{OH} \\ \end{array}$$

OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS

RECORD (14 CITINGS)

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 12 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:657229 CAPLUS

DOCUMENT NUMBER: 136:14976

TITLE: Biomonitoring of urinary tamoxifen and its metabolites

from breast cancer patients using nonaqueous capillary electrophoresis with electrospray mass

spectrometry

AUTHOR(S): Carter, Spencer J.; Li, Xing-Fang; Mackey, John R.;

Modi, Shanu; Hanson, John; Dovichi, Norman J.

CORPORATE SOURCE: Department of Chemistry, University of Alberta,

Edmonton, AB, Can.

SOURCE: Electrophoresis (2001), 22(13), 2730-2736

CODEN: ELCTDN; ISSN: 0173-0835

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal LANGUAGE: English

AB Tamoxifen is an antiestrogen drug used to treat breast cancer.

We have extracted tamoxifen and several of its metabolites from urine of patients with both metastatic (stage IV) and locally confined (stages I, II, and III) breast cancer. Anal. of these metabolites was performed by nonaq. capillary electrophoresis with electrospray-mass spectrometry. Peak heights from extracted ion current electropherograms of the metabolites were used to establish a metabolic profile for each patient. We demonstrate substantial variation among patient profiles, statistically significant differences in the amount of urinary tamoxifen N-oxide found in stages I, II, and III compared to stage IV breast cancer patients, and statistically significant differences in the amount of 3,4-dihydroxytamoxifen found in progressors compared to nonprogressors with metastatic (stage IV) cancer.

IT 65319-40-6, (Z)-3, 4-Dihydroxytamoxifen

RL: PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(urinary tamoxifen and its metabolites from breast cancer patients)

RN 65319-40-6 CAPLUS

CN 1,2-Benzenediol, 4-[(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS

RECORD (19 CITINGS)

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 13 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:242398 CAPLUS

DOCUMENT NUMBER: 135:116418

TITLE: Analysis of tamoxifen and its metabolites in synthetic

gastric fluid digests and urine samples using high-performance liquid chromatography with

electrospray mass spectrometry

AUTHOR(S): Li, X.-F.; Carter, S.; Dovichi, N. J.; Zhao, J. Y.;

Kovarik, P.; Sakuma, T.

CORPORATE SOURCE: University of Alberta, Edmonton, AB, T6G 2G2, Can.

SOURCE: Journal of Chromatography, A (2001), 914(1-2), 5-12

CODEN: JCRAEY; ISSN: 0021-9673

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

AB The authors report on the transformation of tamoxifen at 37° in synthetic gastric fluid as studied by HPLC with triple quadrupole mass spectrometry. The major transformation products detected were (E)-isomer of tamoxifen, metabolite D, and several unidentified components having m/z 404. Addition of pepsin to the gastric fluid inhibited formation of all of these products. The authors analyzed several urine samples from breast cancer patients undergoing tamoxifen treatment. Metabolite D was identified in the urine samples and in the gastric fluid digest at a retention time of 22.0 min eluting from a reversed-phase HPLC column. Although several metabolites were found in all the urine samples of patients, some metabolites were detected in one sample but not others, suggesting tamoxifen metabolism varies in patients.

IT 81992-84-9

RL: ANT (Analyte); ANST (Analytical study)
(anal. of tamoxifen and its metabolites in synthetic gastric fluid
digests and urine samples using high-performance liquid chromatog. with
electrospray mass spectrometry)

RN 81992-84-9 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD

(2 CITINGS)

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 14 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:828028 CAPLUS

DOCUMENT NUMBER: 134:127813

TITLE: Substrate Competitive Inhibitors of IGF-1 Receptor

Kinase

AUTHOR(S): Blum, Galia; Gazit, Aviv; Levitzki, Alexander CORPORATE SOURCE: Department of Biological Chemistry, Alexander

Silberman Institute of Life Sciences Department of

Organic Chemistry, Institute of Chemistry The Hebrew University of Jerusalem, Jerusalem, 91904, Israel

SOURCE: Biochemistry (2000), 39(51), 15705-15712

CODEN: BICHAW; ISSN: 0006-2960

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

AΒ IGF-1 and its receptor play a pivotal role in many cancers, and therefore, IGF-1R is an attractive target for the design of inhibitors. In this communication, we report on a number of lead compds. for inhibitors of the isolated IGF-1R kinase. The search for these compds. utilized two novel in vitro assays and was aided by the knowledge of the three-dimensional structure of the insulin receptor kinase domain, which is 84% homologous to the IGF-1R kinase domain. The most potent inhibitor found in these assays was tyrphostin AG 538, with an IC50 = 400 nM. In computer modeling, AG 538 was placed in the kinase domain of the insulin receptor and was able to sit in place of tyrosines 1158 and 1162, which undergo autophosphorylation. Exptl. it is indeed found that AG 538 does not compete with ATP but competes with the IGF-1R substrate. We prepared I-OMe AG 538, which is more hydrophobic and less sensitive to oxidation than AG 538. Both AG 538 and I-OMe AG 538 inhibit IGR-1R autophosphorylation in intact cells in a dose-dependent manner but I-OMe-AG 538 is superior, probably because of its enhanced hydrophobic nature. Both compds. inhibit the activation of the downstream targets PKB and Erk2. These findings suggest that AG 538 and I-OMe-AG 538 can serve as a lead compound for the development of substrate competitive inhibitors of the IGF-1R. The possible advantage of substrate competitive inhibitors vis-a-vis ATP competitive inhibitors is discussed.

IT 136273-05-7, AG 1233

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); BIOL (Biological study)
(substrate competitive inhibitors of IGF-1 receptor kinase)
RN 136273-05-7 CAPLUS
CN 1,2-Benzenediol, 4,4'-(1E)-1,2-ethenediylbis- (CA INDEX NAME)

Double bond geometry as shown.

IT 321919-11-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (substrate competitive inhibitors of IGF-1 receptor kinase)

RN 321919-11-3 CAPLUS

CN Benzeneacetonitrile, 3,4-dihydroxy- α -[(4-hydroxy-3-iodo-5-methoxyphenyl)methylene]-, (α Z)- (CA INDEX NAME)

Double bond geometry as shown.

OS.CITING REF COUNT: 89 THERE ARE 89 CAPLUS RECORDS THAT CITE THIS

RECORD (89 CITINGS)

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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LAST RELOADED: Jul 24, 2009 (20090724/UP).

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http://www.cas.org/support/stngen/stndoc/properties.html

=> S 321919-11-3/RN

L16 1 321919-11-3/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND SET COMMAND COMPLETED

=> D L16 SQIDE 1-

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L16 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2009 ACS on STN

RN 321919-11-3 REGISTRY

CN Benzeneacetonitrile, 3,4-dihydroxy- α -[(4-hydroxy-3-iodo-5-methoxyphenyl)methylene]-, (α Z)- (CA INDEX NAME)

FS STEREOSEARCH

MF C16 H12 I N O4

SR CA

LC STN Files: CA, CAPLUS

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CAPILLS (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND SET COMMAND COMPLETED

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=> fil reg COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 4.45 611.07 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -27.88

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http://www.cas.org/support/stngen/stndoc/properties.html

=> s ag 538 104312 AG 152 AGS 104457 AG (AG OR AGS) 11188 538 L17 3 AG 538 (AG(W)538)

=> d tot

L17 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2009 ACS on STN

RN 1094048-77-7 REGISTRY

ED Entered STN: 16 Jan 2009

CN Benzenepropanenitrile, 3,4-dihydroxy- α -[(4-hydroxy-3-iodo-5-methoxyphenyl)methylene]- β -oxo-, (α E)- (CA INDEX NAME) OTHER NAMES:

CN I-OMe-tyrphostin AG 538

FS STEREOSEARCH

MF C17 H12 I N O5

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L17 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2009 ACS on STN

RN 875283-46-8 REGISTRY

ED Entered STN: 27 Feb 2006

CN Benzenepropanenitrile, α -[(3,4-dihydroxyphenyl)methylene]-3,4-dihydroxy- β -oxo- (CA INDEX NAME)

OTHER NAMES:

CN Tyrphostin AG 538

MF C16 H11 N O5

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L17 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2009 ACS on STN

RN 133550-18-2 REGISTRY

ED Entered STN: 03 May 1991

CN Benzenepropanenitrile, α -[(3,4-dihydroxyphenyl)methylene]-3,4-dihydroxy- β -oxo-, (α E)- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzenepropanenitrile, $\alpha-[(3,4-dihydroxyphenyl)methylene]-3,4-dihydroxy-<math>\beta$ -oxo-, (E)-

OTHER NAMES:

CN AG 538

FS STEREOSEARCH

MF C16 H11 N O5

CI COM

SR CA

LC STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM, TOXCENTER, USPATFULL

(*File contains numerically searchable property data)

Double bond geometry as shown.

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24 REFERENCES IN FILE CA (1907 TO DATE)
24 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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FILE COVERS 1907 - 29 Jul 2009 VOL 151 ISS 5
FILE LAST UPDATED: 28 Jul 2009 (20090728/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

CAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2009.

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=> d

L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2009 ACS on STN

AN 2000:828028 CAPLUS

DN 134:127813

TI Substrate Competitive Inhibitors of IGF-1 Receptor Kinase

AU Blum, Galia; Gazit, Aviv; Levitzki, Alexander

CS Department of Biological Chemistry, Alexander Silberman Institute of Life Sciences Department of Organic Chemistry, Institute of Chemistry The Hebrew University of Jerusalem, Jerusalem, 91904, Israel

SO Biochemistry (2000), 39(51), 15705-15712 CODEN: BICHAW; ISSN: 0006-2960

PB American Chemical Society

DT Journal

LA English

OSC.G 89 THERE ARE 89 CAPLUS RECORDS THAT CITE THIS RECORD (89 CITINGS)

RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> FIL REGISTRY

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ENTRY SESSION 0.00 -27.88

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```
=> s ag 1233
        104312 AG
           152 AGS
        104457 AG
                 (AG OR AGS)
          3279 1233
L19
             1 AG 1233
                 (AG(W)1233)
=> d
L19 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2009 ACS on STN
    136273-05-7 REGISTRY
ED
    Entered STN: 20 Sep 1991
    1,2-Benzenediol, 4,4'-(1E)-1,2-ethenediylbis- (CA INDEX NAME)
OTHER CA INDEX NAMES:
    1,2-Benzenediol, 4,4'-(1,2-\text{ethenediyl}) bis-, (E)-
CN
OTHER NAMES:
    AG 1233
CN
FS
     STEREOSEARCH
    C14 H12 O4
MF
SR
     CA
LC
     STN Files:
                  CA, CAPLUS, CASREACT, TOXCENTER
```

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 11 REFERENCES IN FILE CA (1907 TO DATE)
- 11 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=>

Connection closed by remote host